SUPLEMENTARY MATERIAL

Hydrodefluorination of Functionalized Fluoroaromatics with Triethylphosphine: A theoretical and Experimental Study.

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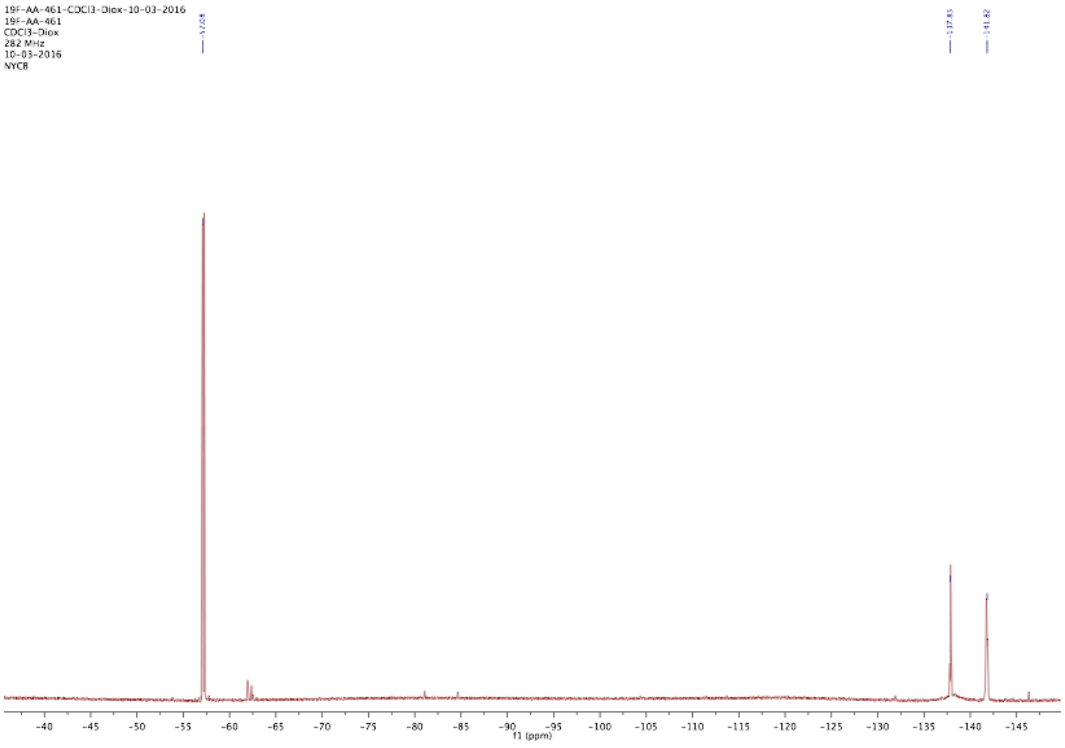

Figure S1. ^{19}F NMR of 2,3,5,6-Tetrafluorotoluene (3).

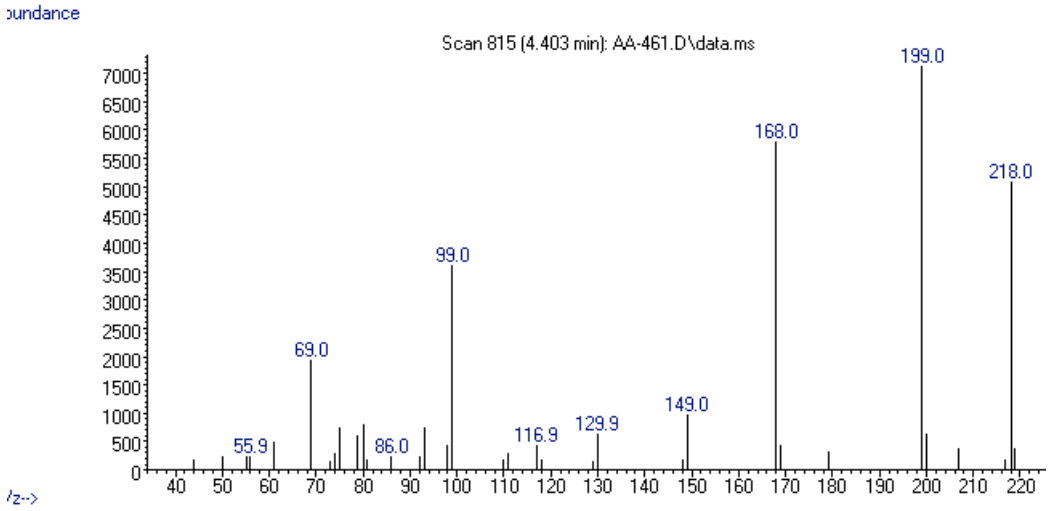

Figure S2. Mass spectrum of 2,3,5,6-Tetrafluorotoluene (3).

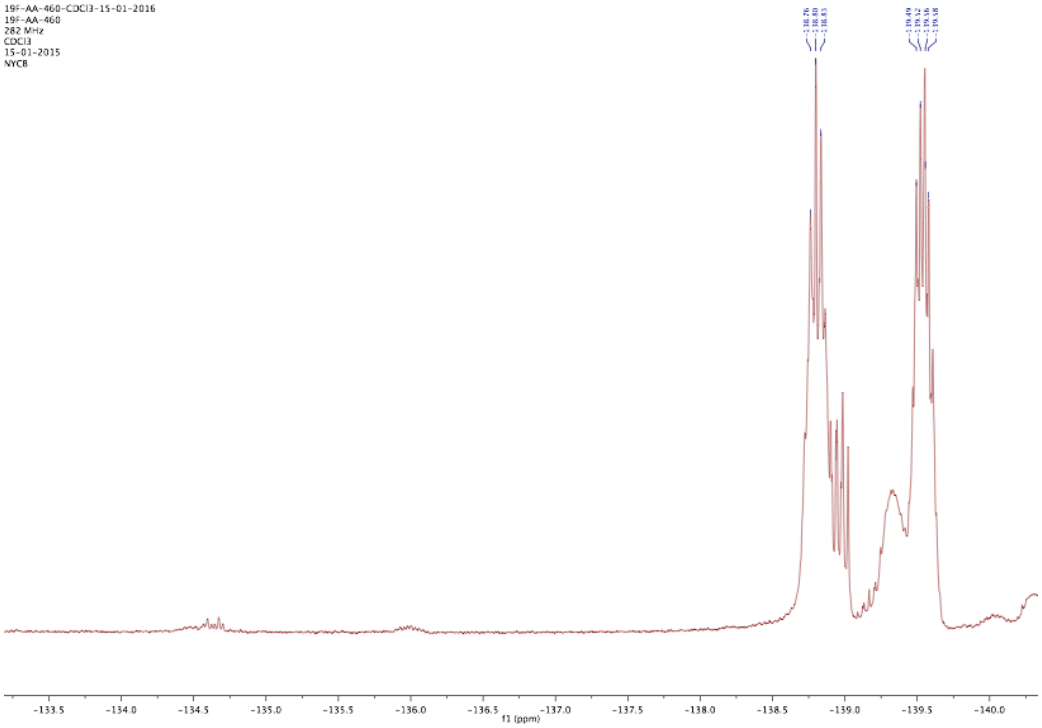

Figure S3. ^{19}F NMR of 2,2',3,3',5,5',6,6'-octafluoro-1,1'-biphenyl (4).

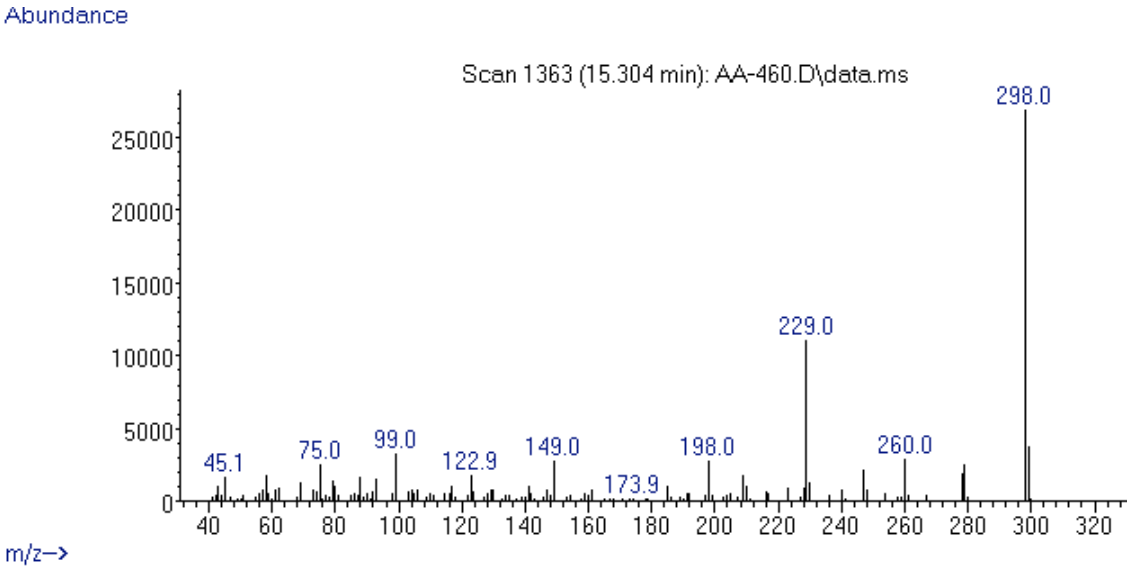

Figure S4. Mass Spectrum of 2,2',3,3',5,5',6,6'-octafluoro-1,1'-biphenyl (4).

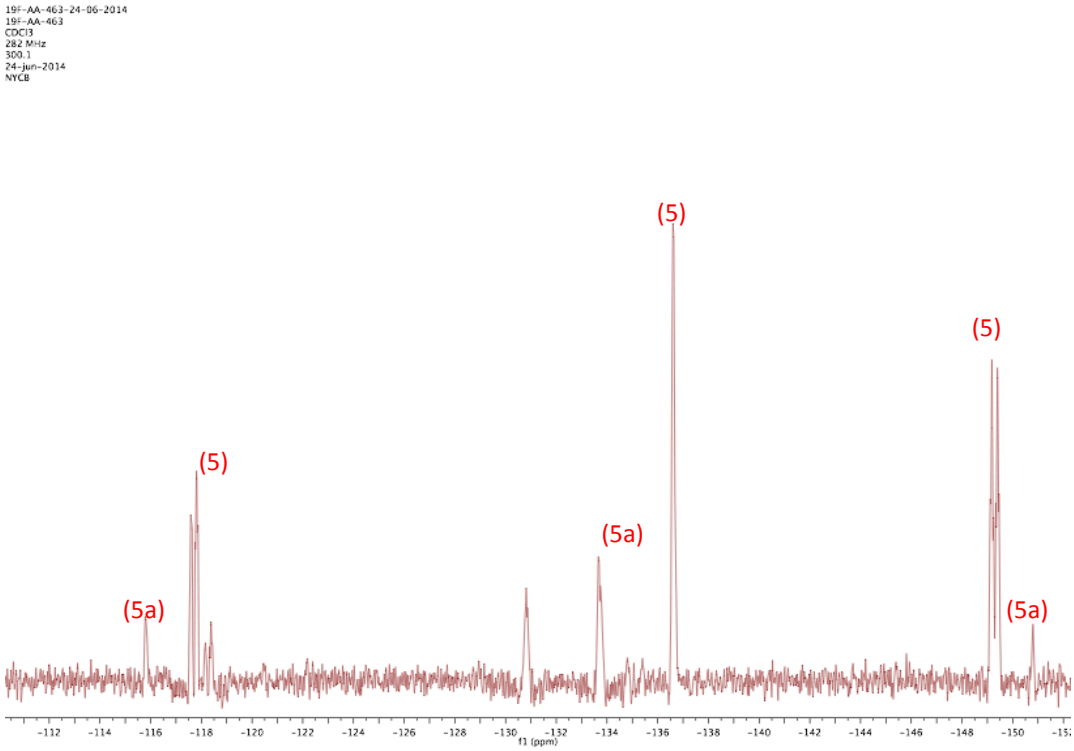

Figure S5. ^{19}F NMR of Hexafluoronaphtalene (5) and (5a).

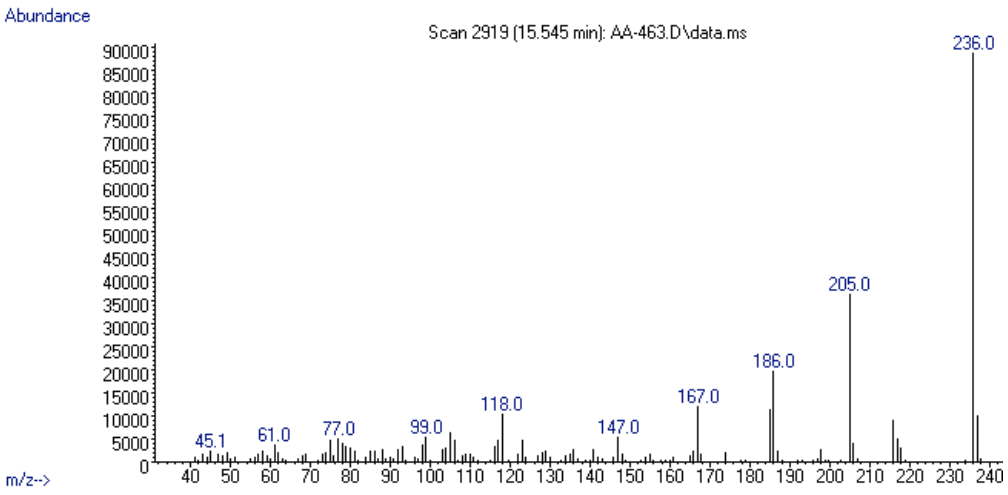

Figure S6. Mass Spectrum of 1,2,4,5,6,8,-hexafluoronaphtalene (5).

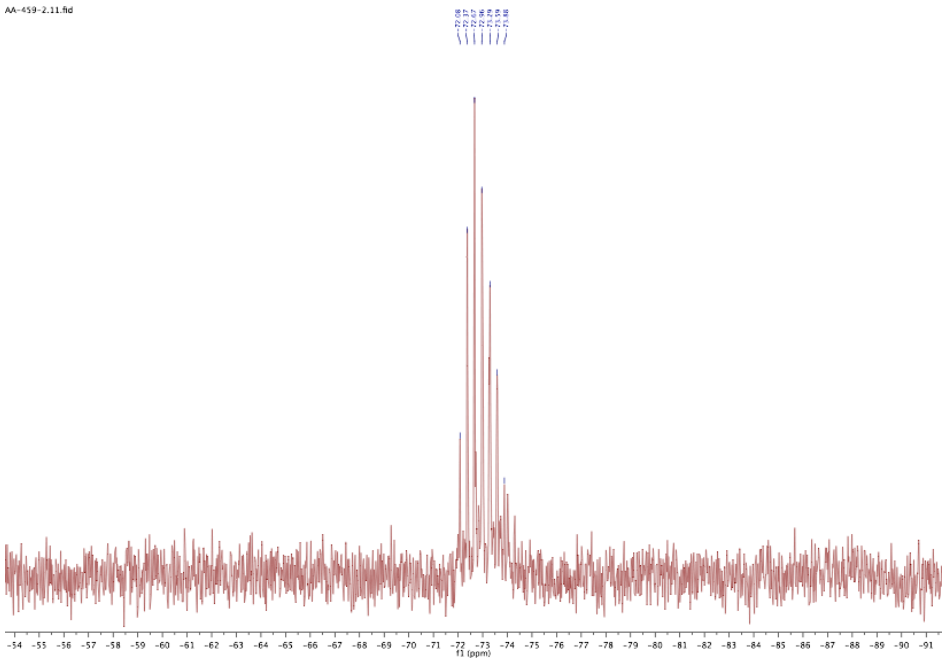

Figure S7. $^{31}P\{^{1}H\}$ NMR of Tris(2,3,5,6-Tetrafluorophenylphosphine) (6).

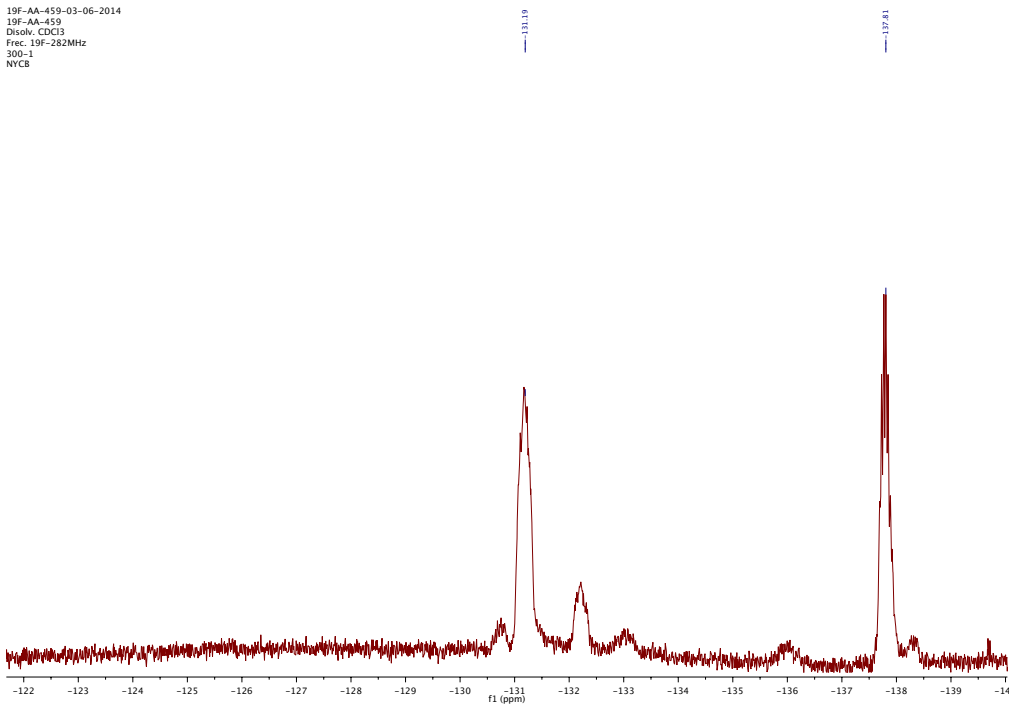

Figure S8. ^{19}F NMR of Tris(2,3,5,6-Tetrafluorophenylphosphine) (6).

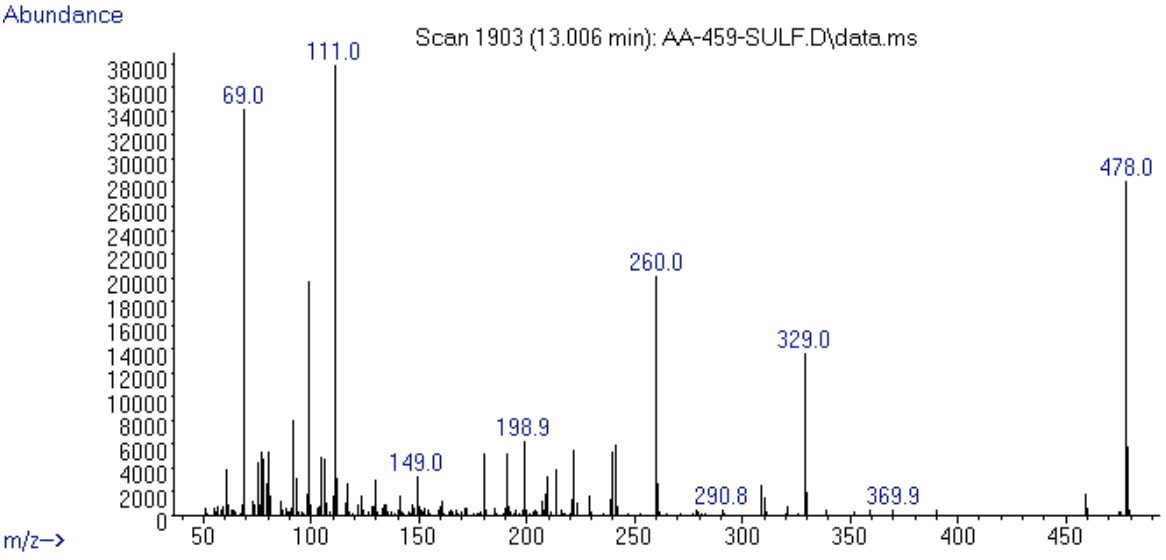

Figure S9. Mass Spectrum of Tris(2,3,5,6-Tetrafluorophenylphosphine) (6).

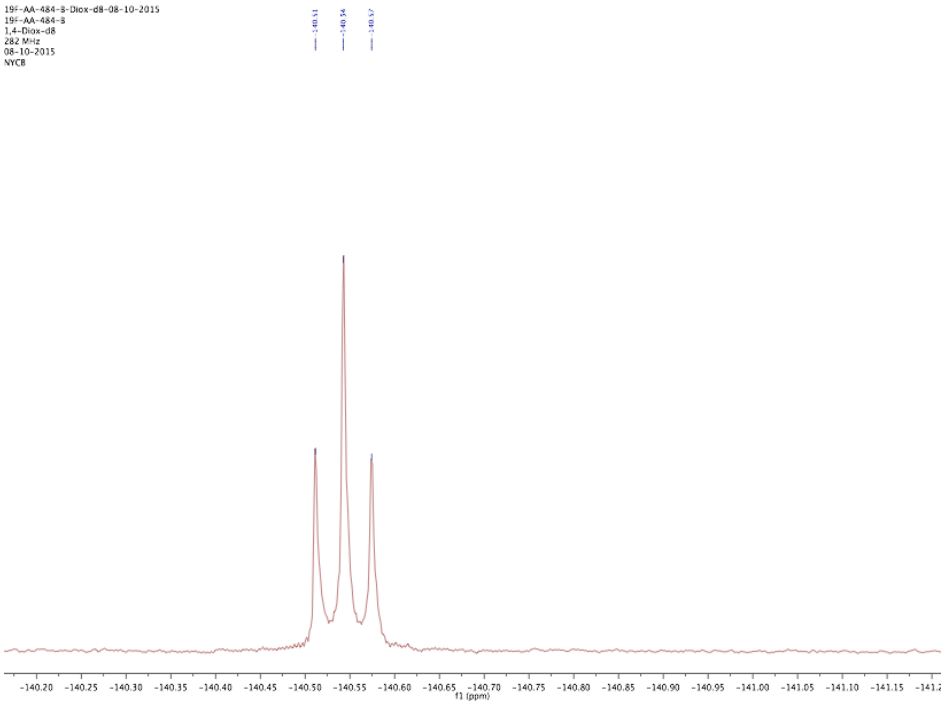

Figure S10. ^{19}F NMR of 2,3,5,6-Tetrafluorobenzene (7).

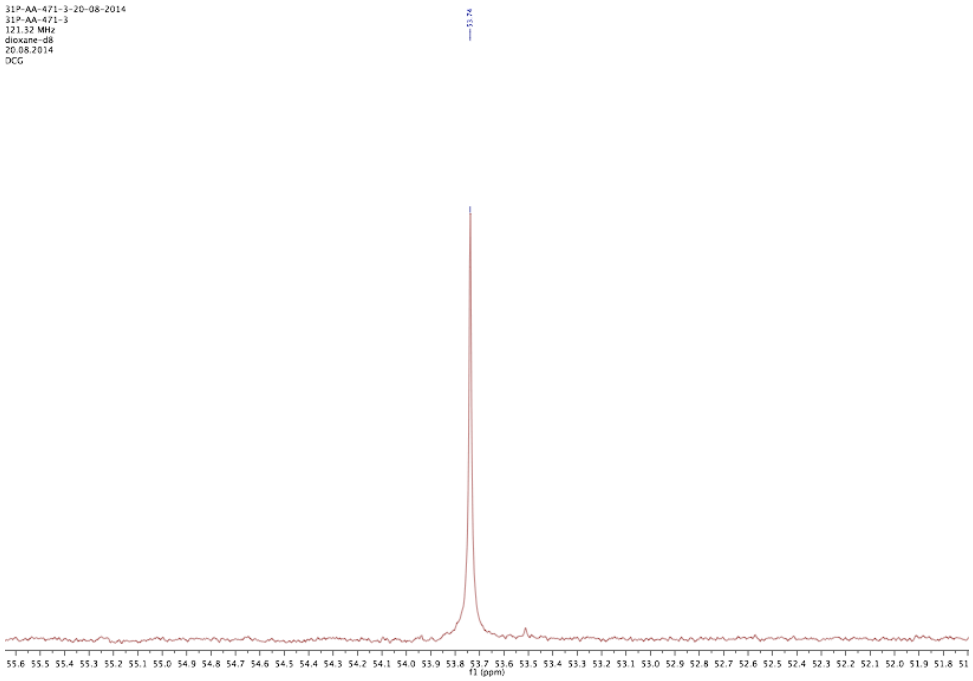

Figure S11. $^{31}P\{^{1}H\}$ NMR of $Et_3P{=}S$ (7b).

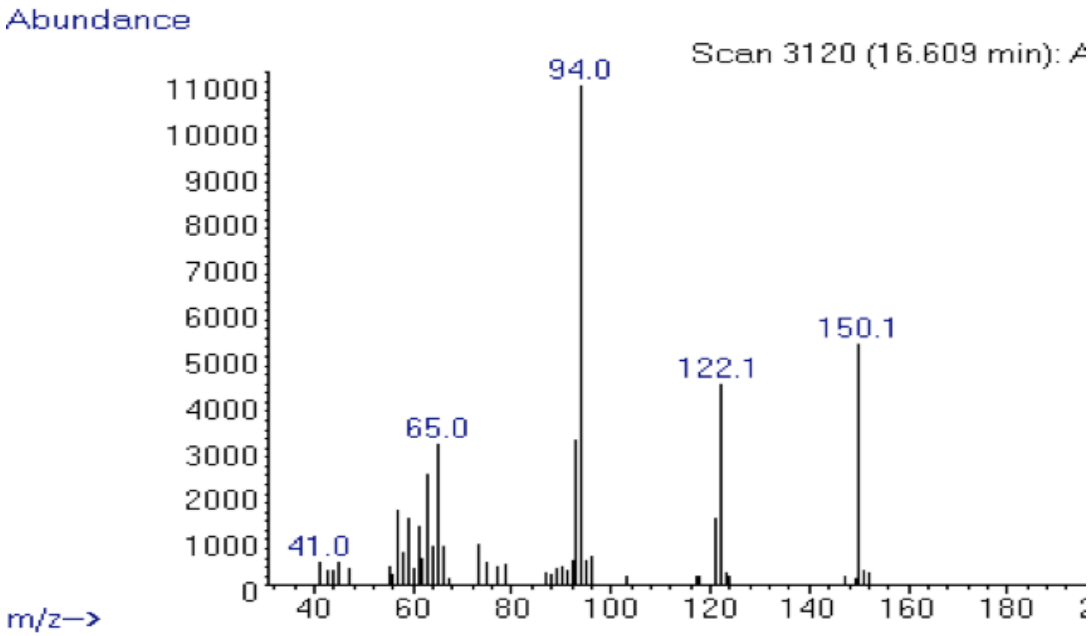

Figure S12. Mass Spectrum of $Et_3P{=}S$ (7b).

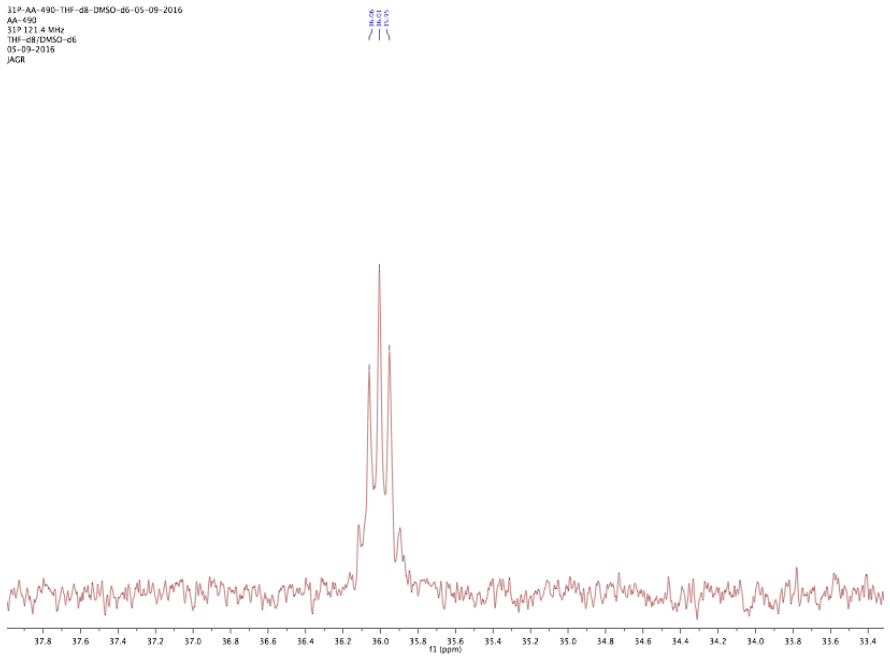

Figure S13. $^{31}P\{^{1}H\}$ NMR of 2,3,5,6-Tetrafluoro_4-(triethylphosphonio)benzenethiolate (2).

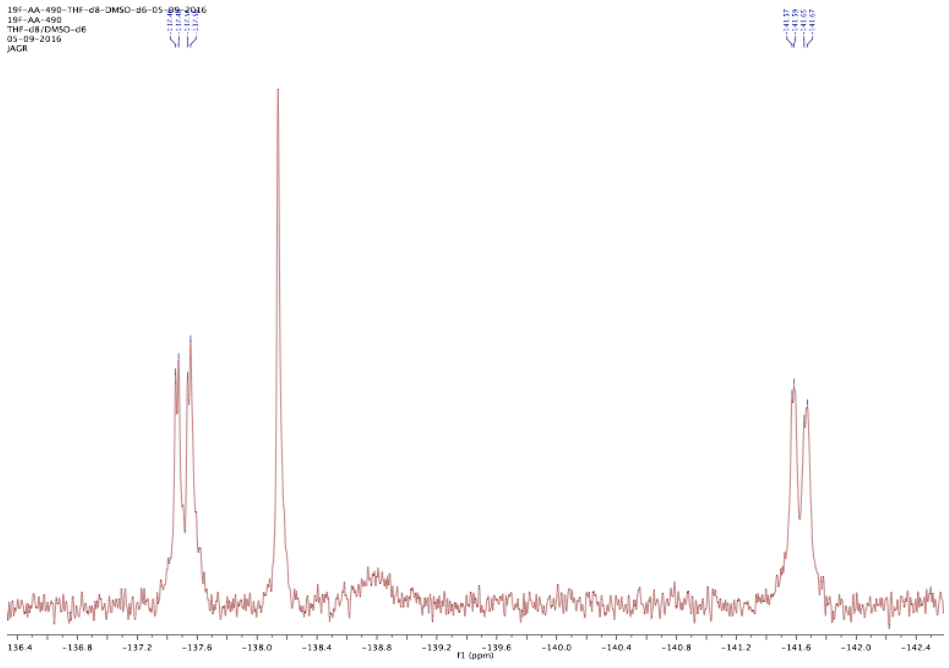

Figure S14. ^{19}F NMR of 2,3,5,6-Tetrafluoro-4-(triethylphosphonio)benzenethiolate (2).

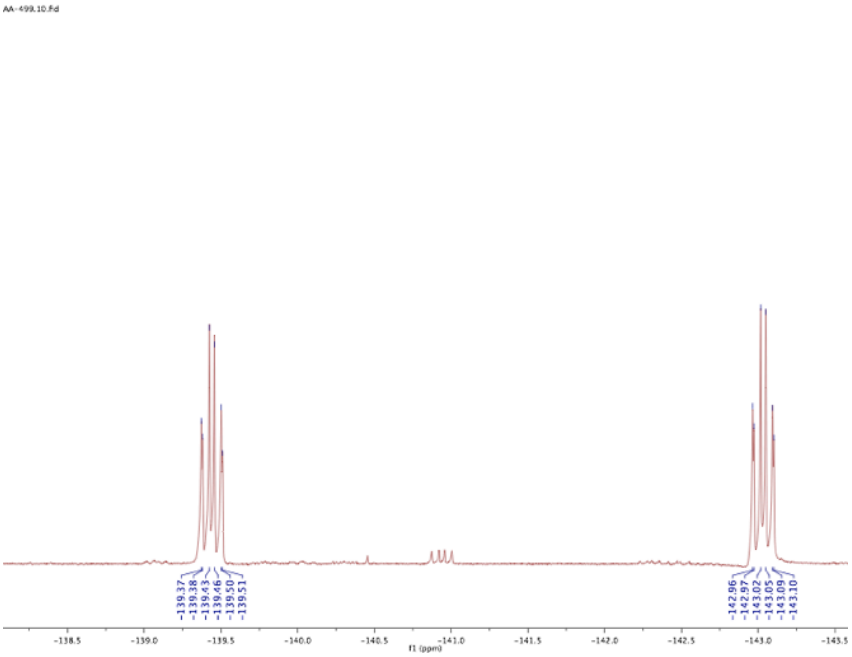

Figure S15. ^{19}F NMR of 2,3,5,6,-Tetrafluorobenzamide (10).

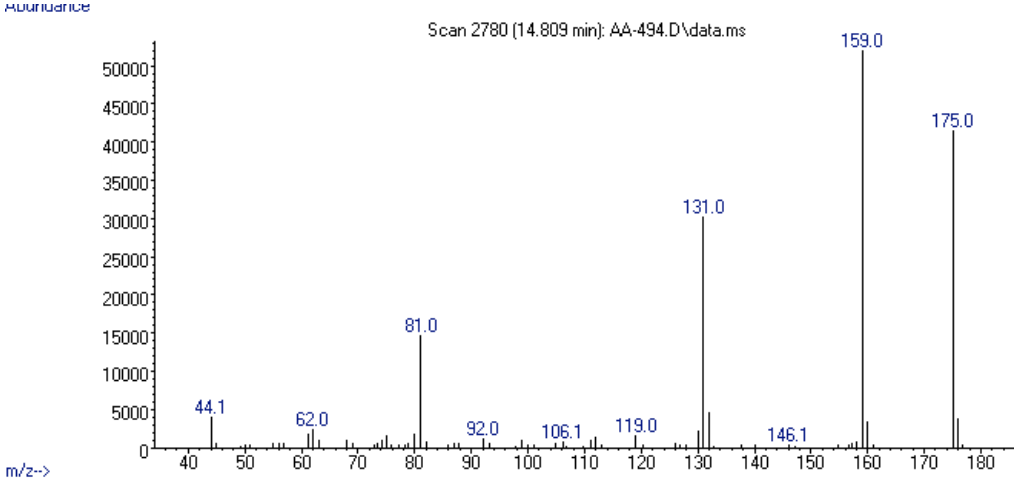

Figure S16. Mass Spectrum of 2,3,5,6-Tetrafluorobenzamide (10).

Deuterium Labelling Studies

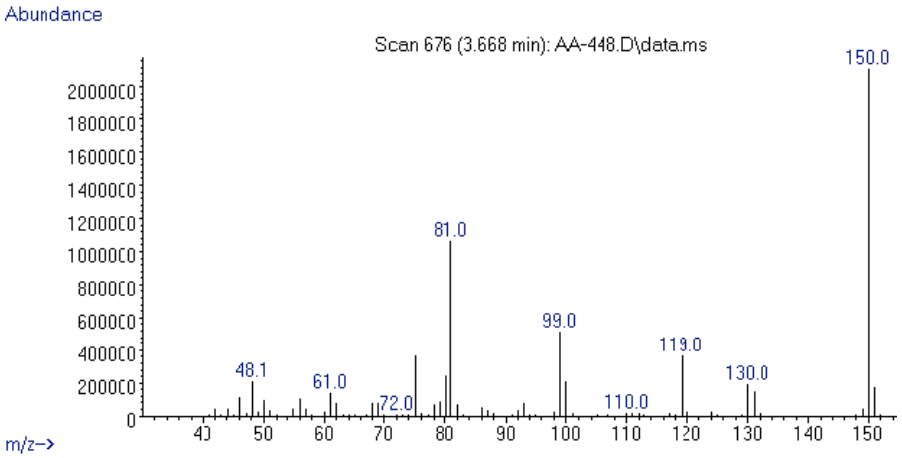

Figure S17. Mass Spectrum of 2,3,5,6-Tetrafluorobenzene (7) without D_2O. M^+ = 150 m/z

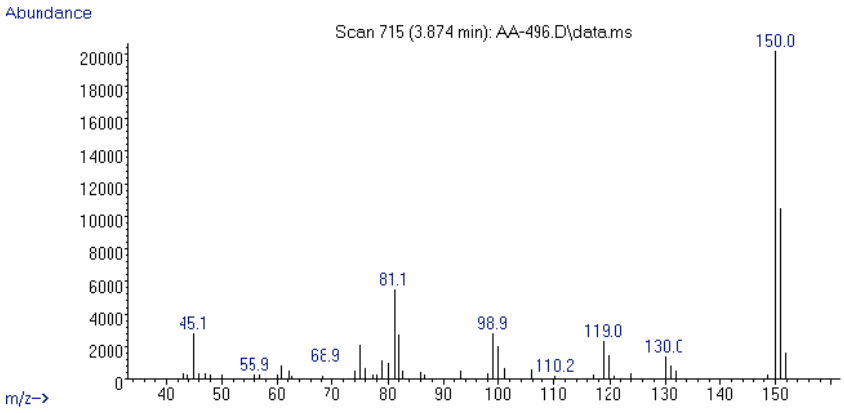

Figure S18. Mass Spectrum of 2,3,5,6-Tetrafluorobenzene (7) with D_2O. M^+ = 151 m/z.

The white solids were analized by multinuclear NMR and ethyl phosphonic acid ($^{31}P\{^1H\}$ at δ = 39.6 (s))[1] as principal product was detected, along with PEt_3=O (a) and remanent PEt_3 (c) .

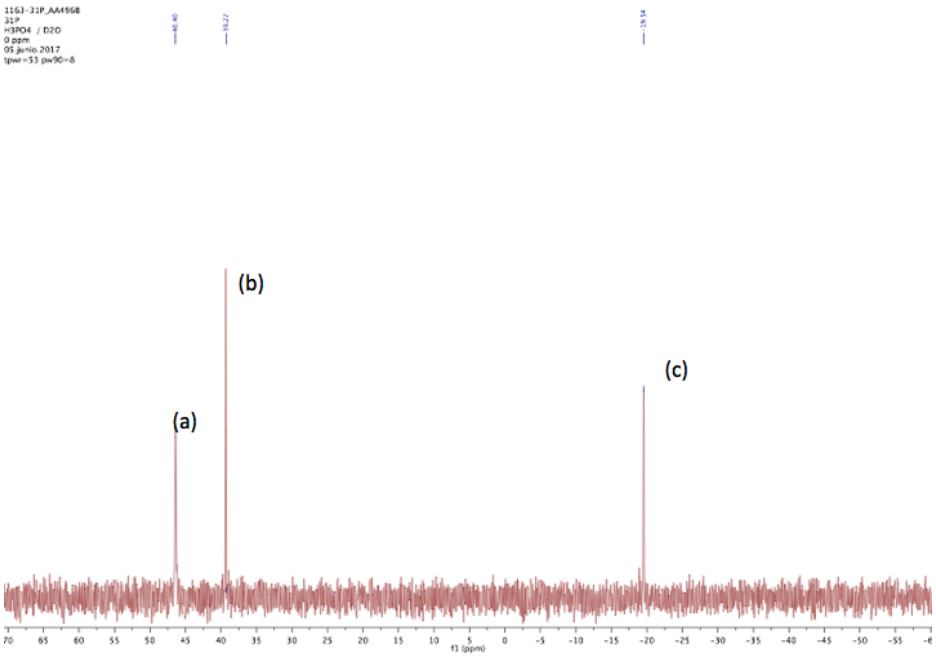

Figure S19. $^{31}P\{^{1}H\}$ NMR of Phosphorous containing products. Ethylphosphonic acid (b) as major product.

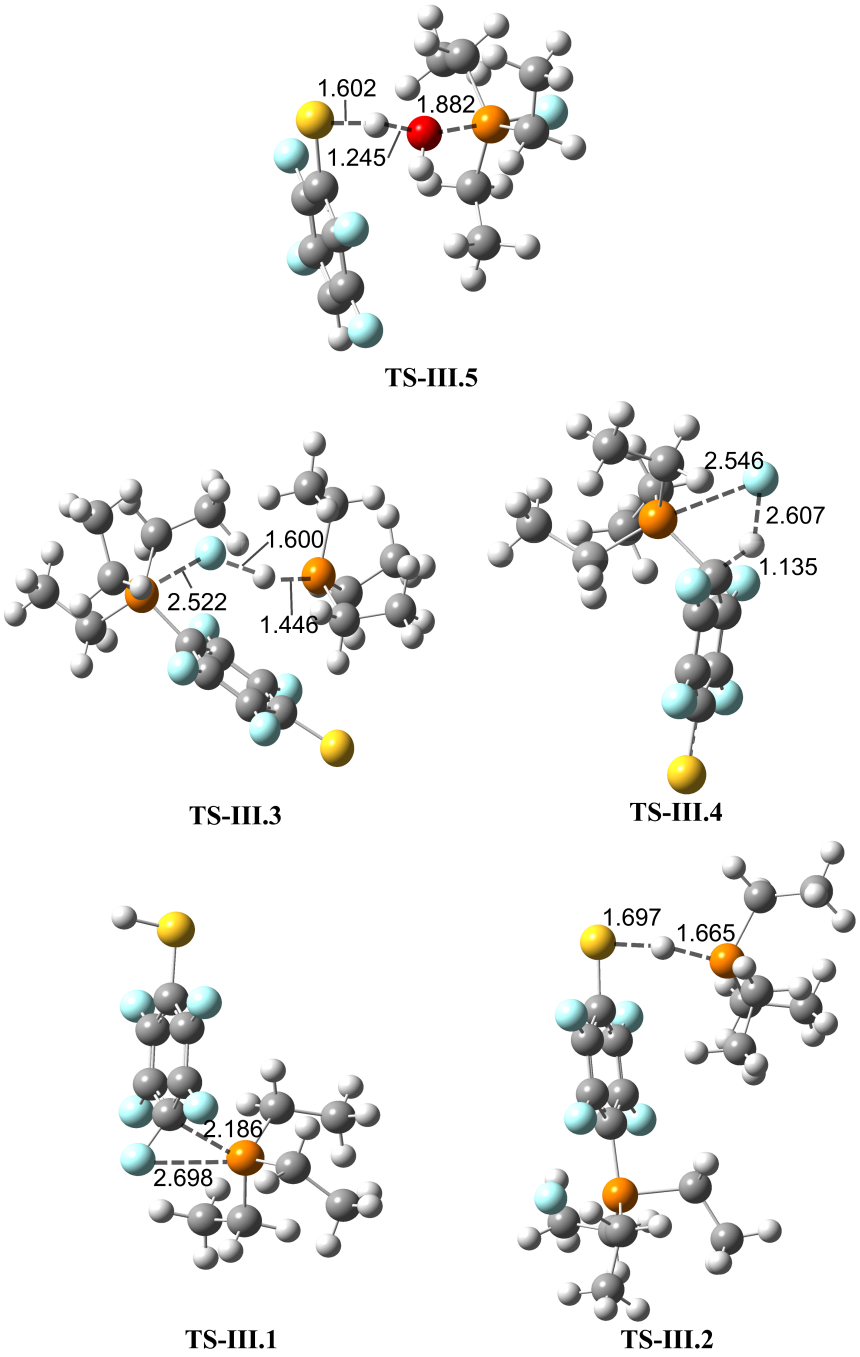

Figure S20. Transition States of Mechanism III. Relevant distances are shown in Å.

°

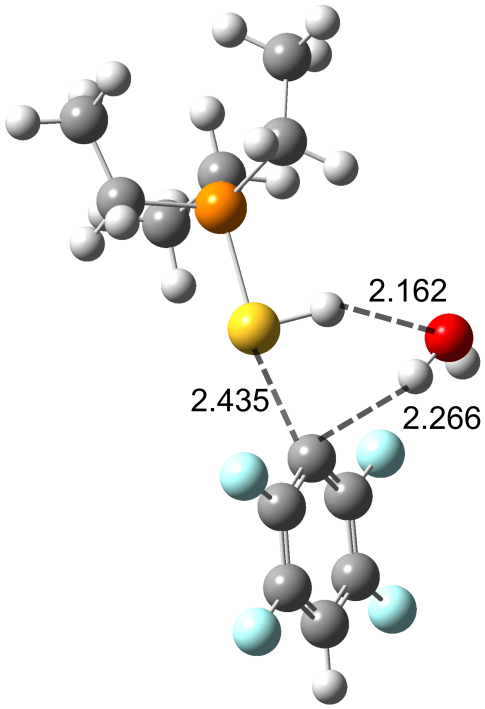

Figure S21. Transition State of Mechanism IV. Relevant distances are shown in Å.

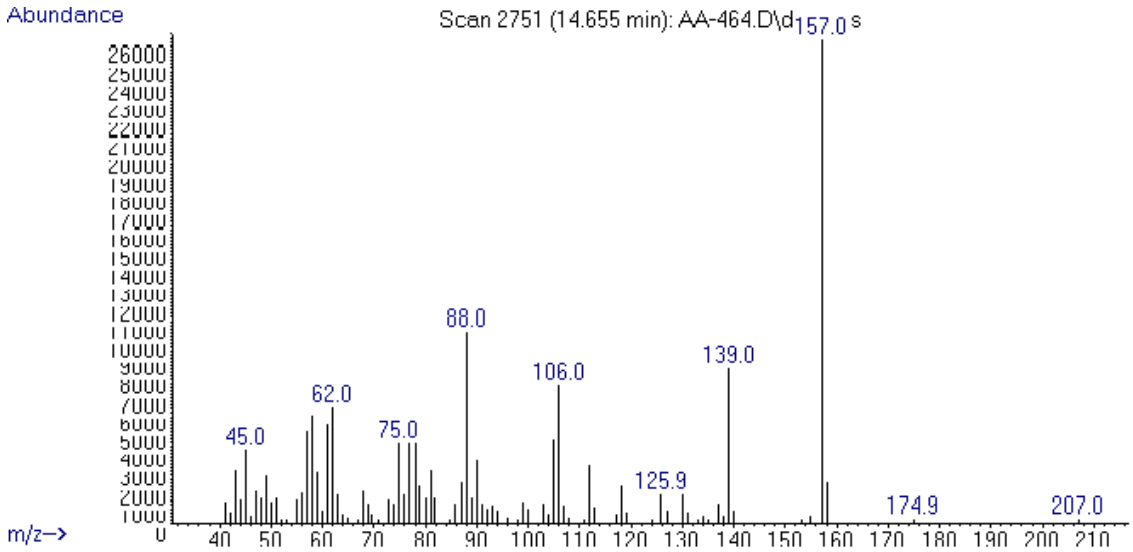

Figure S22. MS compound **9.**

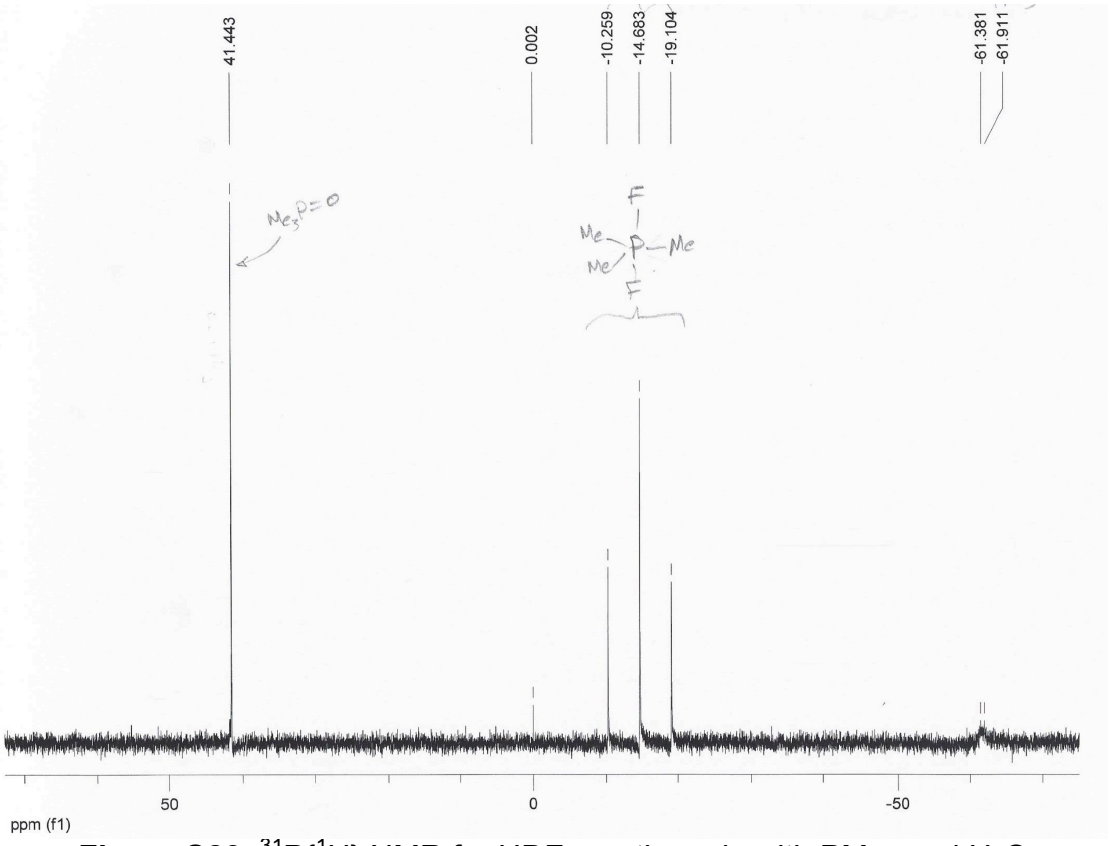

Figure S23. $^{31}P\{^{1}H\}$ NMR for HDF reaction mix with PMe_3 and H_2O

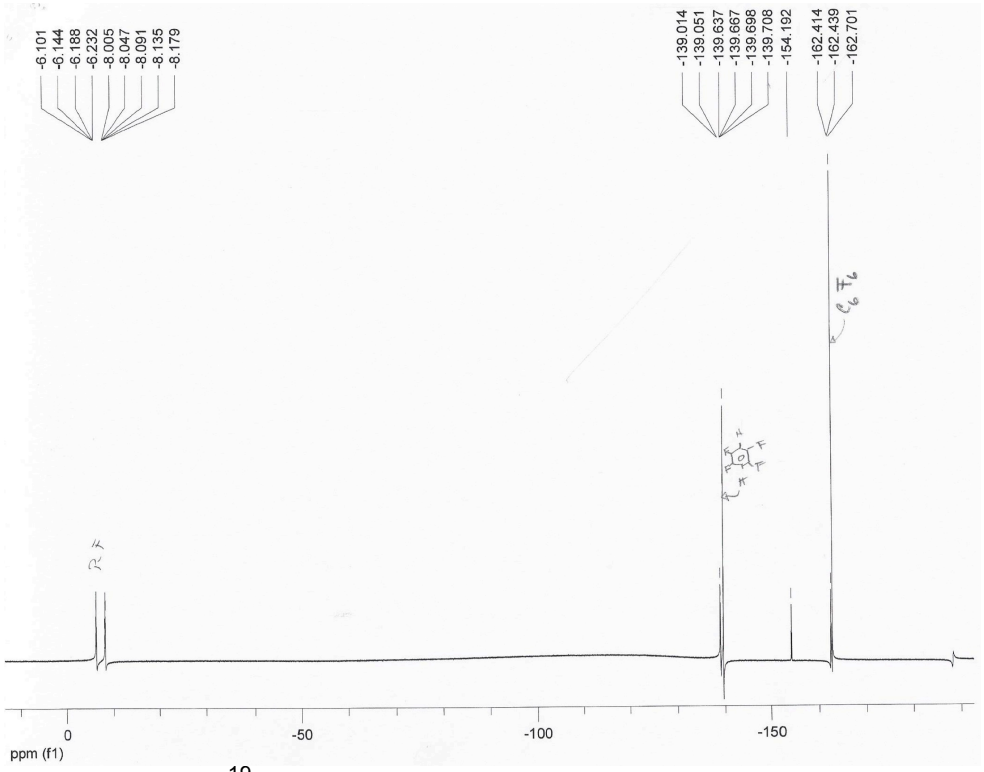

Figure S24. ^{19}F NMR for HDF reaction mix with PMe_3 and H_2O

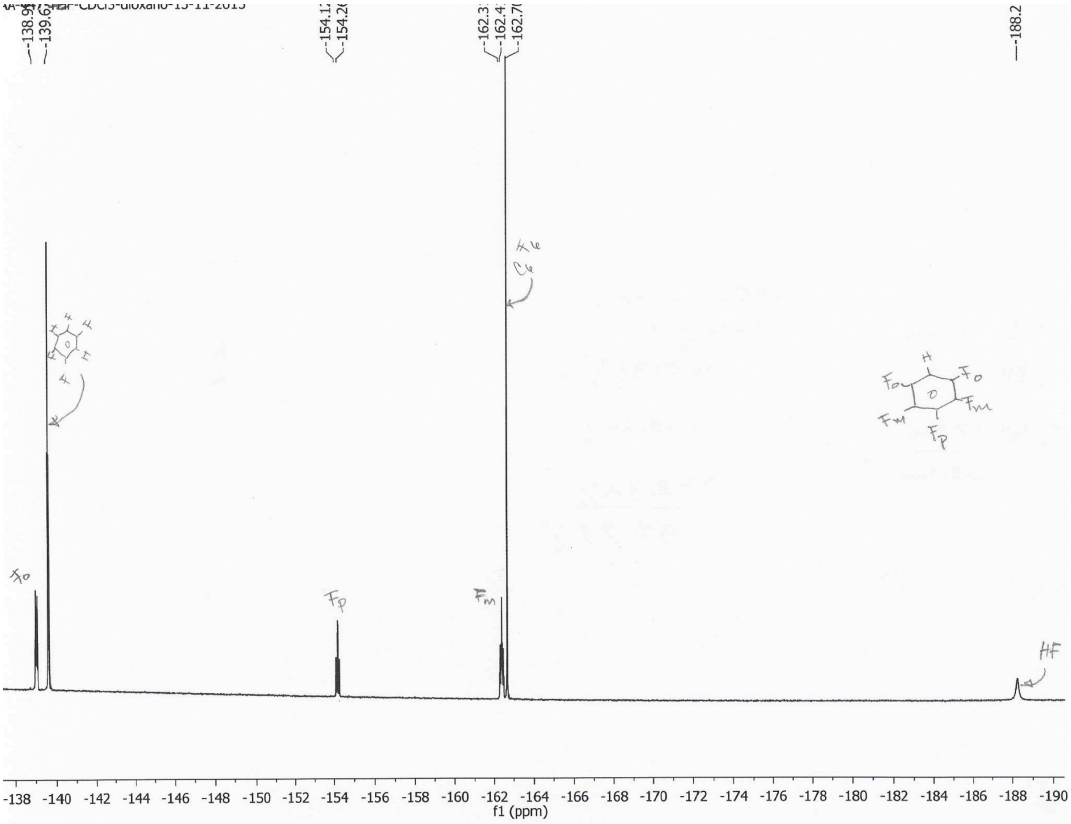

Figure S25. ^{19}F NMR for HDF reaction mix with PMe_3 and H_2O (high field expansion)

Table S1. Crystal data and structure refinement for compound **2**

Identification code	compound **2**|	
Empirical formula	C12 H15 F4 P S	
Formula weight	298.27	
Temperature	130(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$Pca2_1$	
Unit cell dimensions	a = 12.1337(12) Å	α= 90°.
	b = 10.3273(10) Å	β= 90°.
	c = 10.8935(12) Å	γ = 90°.
Volume	1365.0(2) $Å^3$	
Z	4	
Density (calculated)	1.451 Mg/m^3	
Absorption coefficient	0.380 mm^{-1}	
F(000)	616	
Crystal size	0.180 x 0.140 x 0.060 mm^3	
Theta range for data collection	3.741 to 29.605°.	
Index ranges	-16<=h<=16, -14<=k<=12, -14<=l<=13	
Reflections collected	5780	
Independent reflections	2905 [R(int) = 0.0563]	
Completeness to theta = 25.242°	99.7 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2905 / 1 / 166	
Goodness-of-fit on F^2	1.005	
Final R indices [I>2sigma(I)]	R1 = 0.0483, wR2 = 0.0921	
R indices (all data)	R1 = 0.0729, wR2 = 0.1046	
Absolute structure parameter	-0.03(11)	
Largest diff. peak and hole	0.486 and -0.407 e.$Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å2x 103) for compound **2**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	4804(4)	5969(4)	5026(5)	21(1)
C(2)	5499(4)	4982(4)	4606(4)	20(1)
C(3)	5268(3)	3700(4)	4781(5)	19(1)
C(4)	4323(4)	3242(4)	5391(4)	20(1)
C(5)	3633(4)	4240(5)	5799(5)	22(1)
C(6)	3859(4)	5516(4)	5637(5)	22(1)
C(7)	5020(4)	8430(5)	6362(4)	20(1)
C(8)	5974(4)	7988(5)	7166(5)	27(1)
C(9)	3807(4)	8344(5)	4074(5)	24(1)
C(10)	3575(4)	7735(6)	2834(5)	36(1)
C(11)	6230(4)	8061(5)	4036(5)	21(1)
C(12)	6404(4)	9522(5)	3931(5)	29(1)
F(1)	6434(2)	5300(3)	3997(3)	31(1)
F(2)	6003(2)	2831(3)	4327(3)	32(1)
F(3)	2690(2)	3938(3)	6393(3)	33(1)
F(4)	3127(2)	6399(3)	6069(3)	36(1)
P(1)	4987(1)	7685(1)	4868(1)	18(1)
S(1)	4018(1)	1635(1)	5603(1)	24(1)

Table S3. Bond lengths [Å] and angles [°] for compound 2.

C(1)-C(2)	1.400(6)
C(1)-C(6)	1.405(6)
C(1)-P(1)	1.795(5)
C(2)-F(1)	1.355(5)
C(2)-C(3)	1.366(6)
C(3)-F(2)	1.359(5)
C(3)-C(4)	1.408(6)
C(4)-C(5)	1.401(7)

C(4)-S(1)	1.716(5)
C(5)-F(3)	1.351(5)
C(5)-C(6)	1.358(6)
C(6)-F(4)	1.357(5)
C(7)-C(8)	1.522(7)
C(7)-P(1)	1.801(5)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900

C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-C(10)	1.516(7)
C(9)-P(1)	1.806(4)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-C(12)	1.528(7)
C(11)-P(1)	1.802(5)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(2)-C(1)-C(6)	113.9(4)
C(2)-C(1)-P(1)	127.8(4)
C(6)-C(1)-P(1)	118.3(3)
F(1)-C(2)-C(3)	118.3(4)
F(1)-C(2)-C(1)	119.2(4)
C(3)-C(2)-C(1)	122.4(4)
F(2)-C(3)-C(2)	117.1(4)
F(2)-C(3)-C(4)	119.0(4)
C(2)-C(3)-C(4)	123.9(4)
C(5)-C(4)-C(3)	112.9(4)
C(5)-C(4)-S(1)	122.7(4)
C(3)-C(4)-S(1)	124.3(3)
F(3)-C(5)-C(6)	117.3(4)
F(3)-C(5)-C(4)	119.2(4)
C(6)-C(5)-C(4)	123.5(4)
F(4)-C(6)-C(5)	118.3(4)
F(4)-C(6)-C(1)	118.4(4)

C(5)-C(6)-C(1)	123.3(4)
C(8)-C(7)-P(1)	114.1(3)
C(8)-C(7)-H(7A)	108.7
P(1)-C(7)-H(7A)	108.7
C(8)-C(7)-H(7B)	108.7
P(1)-C(7)-H(7B)	108.7
H(7A)-C(7)-H(7B)	107.6
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(10)-C(9)-P(1)	114.7(3)
C(10)-C(9)-H(9A)	108.6
P(1)-C(9)-H(9A)	108.6
C(10)-C(9)-H(9B)	108.6
P(1)-C(9)-H(9B)	108.6
H(9A)-C(9)-H(9B)	107.6
C(9)-C(10)-H(10A)	109.5
C(9)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(9)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(12)-C(11)-P(1)	111.5(4)
C(12)-C(11)-H(11A)	109.3
P(1)-C(11)-H(11A)	109.3
C(12)-C(11)-H(11B)	109.3
P(1)-C(11)-H(11B)	109.3
H(11A)-C(11)-H(11B)	108.0
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5

H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(1)-P(1)-C(11)	111.4(2)
C(1)-P(1)-C(7)	109.8(2)

C(11)-P(1)-C(7)	110.1(2)
C(1)-P(1)-C(9)	108.7(2)
C(11)-P(1)-C(9)	109.9(2)
C(7)-P(1)-C(9)	106.8(2)

Table S4. Anisotropic displacement parameters ($Å^2$x 10^3)for compound 2. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

A	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	23(2)	15(2)	25(3)	-1(2)	1(2)	0(2)
C(2)	17(2)	18(2)	26(3)	0(2)	2(2)	-1(2)
C(3)	15(2)	18(2)	25(2)	-4(2)	0(2)	5(2)
C(4)	25(2)	14(2)	21(3)	1(2)	-7(2)	0(2)
C(5)	22(2)	19(2)	24(3)	-2(2)	5(2)	-7(2)
C(6)	21(2)	18(2)	27(2)	-5(2)	6(2)	2(2)
C(7)	25(2)	16(2)	19(2)	-3(2)	4(2)	1(2)
C(8)	33(3)	25(3)	22(3)	-5(2)	2(2)	4(2)
C(9)	21(2)	18(3)	32(3)	3(2)	-3(2)	1(2)
C(10)	26(3)	45(4)	38(3)	-12(3)	-5(3)	4(3)
C(11)	21(2)	22(3)	20(3)	3(2)	1(2)	-5(2)
C(12)	27(3)	23(3)	37(3)	0(2)	4(2)	-5(2)
F(1)	23(2)	22(2)	48(2)	-2(1)	18(1)	-2(1)
F(2)	31(2)	16(2)	49(2)	-5(1)	11(1)	5(1)
F(3)	32(2)	23(2)	45(2)	-1(2)	18(1)	-6(1)
F(4)	30(2)	20(2)	57(2)	-5(1)	20(1)	3(1)
P(1)	18(1)	14(1)	21(1)	-2(1)	1(1)	0(1)
S(1)	33(1)	15(1)	25(1)	0(1)	0(1)	-1(1)

Table S5. Total Zero-Point Energies (ZPE) (Hartree), Total Gibbs Energies (Hartree) and Imaginary Frequencies (cm^{-1}) for all species of Mechanism I at 393K. M062X/6-311++G(3df,3pd).

HFB

Species	E_{ZPE}	Gibbs Energy (298 K)	Gibbs Energy (393 K)	Imaginary Frequency
C_6F_6	-827.597605	-827.631212	-827.646092	---
PEt_3	-578.775583	-578.810774	-578.826520	---
TS-I.1	-1406.349336	-1406.398561	-1406.423053	159.17*i*
Int I.A	-1406.419860	-1406.467629	-1406.491437	---
TS-I.2	-1406.304924	-1406.350601	-1406.373431	825.08*i*
Int I.B	-1327.855292	-1327.901700	-1327.924007	---
Ethene	-78.519498	-78.541665	-78.550232	---
TS-I.3.	-1327.752219	-1327.828633	-1327.850987	757.28*i*
C_6F_5H	-728.361908	-728.394981	-728.409313	---
PEt_2F	-599.493178	-599.539753	-599.553652	---

PFP

Species	E_{ZPE}	Gibbs Energy (298 K)	Gibbs Energy (393 K)	Imaginary Frequency
C_5F_5N	-744.428355	-744.461926	-744.476279	---
PEt_3	-578.775583	-578.810774	-578.826520	---
TS-I.1	-1323.191232	-1323.23989	-1323.263714	191.26*i*
Int I.A	-1323.247915	-1323.294514	-1323.317478	---
TS-I.2	-1323.132546	-1323.176995	-1323.198952	820.58*i*
Int I.B	-1244.681474	-1244.726465	-1244.747849	---
Ethene	-78.519498	-78.541665	-78.550232	---
TS-I.3.	-1244.628164	-1244.672118	-1244.693070	883.33*i*
C_5F_4HN	-645.187403	-645.219134	-645.232550	---
PEt_2F	-599.493178	-599.539753	-599.553652	---

Table S6. Total Zero-Point Energies (ZPE) (Hartree), Total Gibbs Energies (Hartree) and Imaginary Frequencies (cm^{-1}) for all species of Mechanism II at 393K. M062X/6-311++G(3df,3pd). Reactants, TS-II.1 and Int II.A are the same as in Mechanism I, but they are included for clarity.

HFB

Species	E_{ZPE}	Gibbs Energy (298 K)	Gibbs Energy (393 K)	Imaginary Frequency
C_6F_6	-827.597605	-827.631212	-827.646092	---
PEt_3	-578.775583	-578.810774	-578.826520	---
H_2O	-76.408421	-76.426711	-76.433919	---
TS-II.1	-1406.349336	-1406.398561	-1406.423053	-159.17*i*
Int II.A	-1406.419860	-1406.467629	-1406.491437	---
TS-II.2	-1482.813573	-1482.867422	-1482.894454	-113.46*i*
Ionic Pair II.1	-1482.815878	-1482.870593	-1482.898111	---
TS-II.3	-1482.815439	-1482.869568	-1482.896519	-68.73*i*
C_6F_5H	-728.361908	-728.394981	-728.409313	---
$PEt_3(F)(OH)$	-754.494550	-754.533266	-754.551081	---

PFB

Species	E_{ZPE}	Gibbs Energy (298 K)	Gibbs Energy (393 K)	Imaginary Frequency
C_6F_5H	-728.361908	-728.394981	-728.409313	---

PEt_3	-578.775583	-578.810774	-578.826520	---
H_2O	-76.408421	-76.426711	-76.433919	---
TS-II.1	-1307.113272	-1307.161205	-1307.184874	-169.38*i*
Int II.A	-1307.180488	-1307.227059	-1307.250116	---
TS-II.2	-1383.570393	-1383.622055	-1383.647969	-124.27*i*
Ionic Pair II.1	-1383.574312	-1383.627788	-1383.654520	---
TS-II.3	-1383.573872	-1383.62484	-1383.650143	-39.73*i*
$C_6F_4H_2$	-629.121958	-629.154512	-629.154512	---
$PEt_3(F)(OH)$	-754.494550	-754.533266	-754.551081	---

PFP

Species	E_{ZPE}	Gibbs Energy (298 K)	Gibbs Energy (393 K)	Imaginary Frequency
C_5F_5N	-744.428355	-744.461926	-744.476279	---
PEt_3	-578.775583	-578.810774	-578.826520	---
H_2O	-76.408421	-76.426711	-76.433919	---
TS-II.1	-1323.191232	-1323.239890	-1323.263714	-191.26*i*
Int II.A	-1323.247915	-1323.294514	-1323.317478	---
TS-II.2	-1383.572533	-1383.624881	-1383.651043	-118.77*i*
Ionic Pair II.1	-1399.645156	-1399.698258	-1399.724754	---
TS-II.3	-1399.644613	-1399.698142	-1399.724454	-41.51*i*
C_5F_4HN	-645.187403	-645.219134	-645.232550	---
$PEt_3(F)(OH)$	-754.494550	-754.533266	-754.551081	---

PFT

Species	E_{ZPE}	Gibbs Energy (298 K)	Gibbs Energy (393 K)	Imaginary Frequency
C_5F_5SH	-1126.551395	-1126.587372	-1126.603312	---
PEt_3	-578.775583	-578.810774	-578.826520	---
H_2O	-76.408421	-76.426711	-76.433919	---
TS-II.1	-1705.304054	-1705.354892	-1705.380269	-180.32*i*
Int II.A	-1705.372270	-1705.421217	-1705.445740	---
TS-II.2	-1781.764807	-1781.818949	-1781.846409	-120.78*i*
Ionic Pair II.1	-1781.766655	-1781.823269	-1781.851591	---
TS-II.3	-1781.766497	-1781.822234	-1781.850065	-104.20*i*
C_5F_4HSH	-1027.312896	-1027.34792	-1027.363245	---
$PEt_3(F)(OH)$	-754.494550	-754.533266	-754.551081	---

Table S7. Total Zero-Point Energies (ZPE) (Hartree), Total Gibbs Energies (Hartree) and Imaginary Frequencies (cm^{-1}) for all species of Mechanism III . M062X/6-311++G(3df,3pd). Reactants, TS-III.1 and Int III.A are the same as in Mechanism I and II, but they are included for clarity.

PFT

Species	E_{ZPE}	Gibbs Energy (298 K)	Gibbs Energy (393 K)	Imaginary Frequency
C_5F_5SH	-1126.551395	-1126.587372	-1126.603312	---
PEt_3	-578.775583	-578.810774	-578.826520	---
H_2O	-76.408421	-76.426711	-76.433919	---
TS-III.1	-1705.304054	-1705.354892	-1705.380269	-180.32*i*
Int III.A	-1705.365774	-1705.414945	-1705.439647	---
TS-III.2	-2284.142403	-2284.205922	-2284.239729	-943.98*i*
Ionic Pair III.1	-2284.151292	-2284.213749	-2284.247290	---
TS-III.3	-2284.145266	-2284.207591	-2284.241016	-177.35*i*

Int III.B	-1604.912948	-1604.96178	-1604.985710	---
HF	-100.440999	-100.457400	-100.463831	---
TS-III.4	-1705.309876	-1705.359654	-1705.384380	-224.78*i*
Ionic Pair III.2	-1705.400280	-1705.450139	-1705.474951	---
TS-III.5	-1781.812057	-1781.864871	-1781.891280	-842.59*i*
C_5F_4HSH	-1027.312896	-1027.347920	-1027.363245	---
$PEt_3(F)(OH)$	-754.494550	-754.533266	-754.551081	---

Table S8. Total Zero-Point Energies (ZPE) (Hartree), Total Gibbs Energies (Hartree) and Imaginary Frequencies (cm^{-1}) for all species of Mechanism IV . M062X/6-311++G(3df,3pd).

TFT

Species	E_{ZPE}	Gibbs Energy (298 K)	Gibbs Energy (393 K)	Imaginary Frequency
C_5F_4HSH	-1027.312896	-1027.347920	-1027.363245	---
PEt_3	-578.775583	-578.810774	-578.826520	---
H_2O	-76.408421	-76.426711	-76.433919	---
Complex IV.1	-1103.725328	-1103.767630	-1103.786814	---
TS-IV.1	-1682.465827	-1682.522465	-1682.550646	-82.98*i*
$C_6F_4H_2$	-629.121958	-629.154512	-629.154512	---
PEt_3S	-977.015126	-977.052155	-977.068985	---

Table S9. Optimized geometries in Cartesian Coordinates (Å) of the intermediates and transition states of Mechanism I. M062X/6-311++G(3df,3pd).

TS-I.1 (HFB)

	Coordinates (Å)		
Atom	X	Y	Z
F	-0.353380	2.356012	-0.665217
C	-1.008022	1.185668	-0.531469
C	-2.178048	1.157179	0.187991
F	-2.691540	2.299009	0.638286
C	-2.830169	-0.036197	0.452604
F	-4.001278	-0.061503	1.097313
C	-2.250513	-1.196357	-0.033817
C	-1.077521	-1.165660	-0.752291
C	-0.331280	0.022645	-0.996705
P	1.567312	-0.088599	-0.043360
F	0.204522	0.118787	-2.301400
F	-2.850778	-2.364993	0.174913
F	-0.544992	-2.329102	-1.172198
C	2.090446	-1.833793	0.116079
C	1.136433	0.531581	1.609903
H	1.913334	-2.294257	-0.854573
H	1.390076	-2.301195	0.810419
C	3.542458	-2.055074	0.543326
H	0.911222	1.591909	1.480185
C	2.161782	0.318363	2.719748
H	0.187404	0.047938	1.856710
H	4.231058	-1.684959	-0.213628
H	3.726424	-3.121064	0.664081
H	3.779861	-1.563974	1.483781
H	3.133246	0.736050	2.457504
H	2.290408	-0.739585	2.939167
H	1.825702	0.807379	3.631990
C	3.025647	0.830430	-0.642541
H	3.823021	0.719902	0.095629
C	2.735799	2.301702	-0.928923
H	3.350473	0.315674	-1.547946
H	2.375458	2.817696	-0.040175
H	1.980063	2.404264	-1.703985
H	3.644681	2.799016	-1.261052

TS-I.1 (PFP)

	Coordinates (Å)		
Atom	X	Y	Z
F	-0.508135	2.365841	-0.881206
C	-1.077481	1.182747	-0.615827
C	-2.137211	1.077631	0.242970
F	-2.639382	2.196424	0.754673
C	-2.187271	-1.138587	0.090962
C	-1.128609	-1.173896	-0.777107
C	-0.444967	0.020068	-1.124482
P	1.591307	-0.089374	-0.106736
F	0.060105	0.090451	-2.391385
F	-2.748736	-2.292284	0.436107
F	-0.650432	-2.333894	-1.246204
C	2.104232	-1.839825	0.096348
C	1.114937	0.525805	1.541591
H	1.930822	-2.325063	-0.863395
H	1.393069	-2.283390	0.795946
C	3.547906	-2.072055	0.54429
H	0.860817	1.579352	1.406598
C	2.124397	0.347391	2.672042
H	0.176121	0.017338	1.778894
H	4.249959	-1.721503	-0.209851
H	3.720334	-3.137508	0.686766
H	3.778319	-1.565618	1.478593
H	3.089214	0.788368	2.423216
H	2.277317	-0.705807	2.899052
H	1.760596	0.831698	3.576373
C	3.089127	0.830156	-0.613247
H	3.867015	0.680213	0.137742
C	2.811947	2.316020	-0.831413
H	3.436450	0.361931	-1.535359
H	2.470632	2.794739	0.085541
H	2.046504	2.463765	-1.590681
H	3.719224	2.822761	-1.153815
N	-2.709831	-0.048595	0.608487

Int I.A (HFB)

	Coordinates (Å)		
Atom	X	Y	Z
F	-1.806002	-1.498147	3.079121
C	-2.04412	-0.908671	1.899192
C	-3.393632	-0.808353	1.584462
F	-4.313742	-1.264655	2.425814
C	-3.784339	-0.236815	0.393667
C	-2.812012	0.224414	-0.474125

C	-1.485623	0.098716	-0.116273
C	-1.026832	-0.455034	1.073419
F	-3.16226	0.772744	-1.630636
F	-0.594348	0.550648	-1.014257
C	1.102299	1.354173	1.148353
C	1.156114	-1.584912	-0.189496
H	0.13764	1.793509	0.921842
H	1.775525	1.553919	0.314594
C	1.66346	1.956739	2.436051
H	1.631726	-2.478573	0.217943
C	2.022972	-1.021158	-1.313957
H	0.178188	-1.87276	-0.56132
H	1.000524	1.77581	3.282178
H	1.758937	3.035179	2.317542
H	2.644603	1.551361	2.669452
H	1.616108	-0.094353	-1.713509
H	2.059226	-1.742524	-2.129736
H	3.037748	-0.839203	-0.973329
C	0.96524	-1.164403	2.953348
H	1.900392	-0.865572	3.417643
C	0.850957	-2.688081	2.936357
H	0.151075	-0.713633	3.508676
H	0.005619	-3.02929	2.339115
H	0.71175	-3.061038	3.949555
H	1.758303	-3.136885	2.534546
P	0.985586	-0.471859	1.267218
F	2.719887	-0.501548	1.339231
F	-5.066476	-0.135284	0.082071

Int I.A (PFP)

	Coordinates (Å)		
Atom	X	Y	Z
F	-1.820575	-1.478325	3.089932
C	-2.034429	-0.901136	1.901491
C	-3.366756	-0.774137	1.526256
F	-4.304247	-1.213844	2.353366
C	-2.825689	0.17702	-0.406577
C	-1.481847	0.085863	-0.112167
C	-1.011942	-0.458954	1.077068
F	-3.209669	0.712824	-1.555974
F	-0.611937	0.54158	-1.026172
C	1.105114	1.353911	1.149527
C	1.168973	-1.58339	-0.18546
H	0.136008	1.78422	0.923919
H	1.773404	1.558112	0.312725
C	1.665181	1.963984	2.434504

H	1.652143	-2.474947	0.217594
C	2.024797	-1.012782	-1.315203
H	0.190122	-1.876615	-0.551037
H	1.006945	1.778944	3.283274
H	1.750404	3.042824	2.313037
H	2.650833	1.56813	2.665273
H	1.607098	-0.090697	-1.714122
H	2.063982	-1.735298	-2.129609
H	3.039619	-0.821084	-0.979705
C	0.972211	-1.171303	2.953757
H	1.909703	-0.891208	3.425306
C	0.828916	-2.69248	2.92725
H	0.162443	-0.709003	3.506851
H	-0.018954	-3.013925	2.322469
H	0.675197	-3.067894	3.937287
H	1.729852	-3.156871	2.528847
P	1.011233	-0.471988	1.272061
F	2.734116	-0.494745	1.344175
N	-3.761281	-0.24704	0.402736

TS-I.2 (HFB)

	Coordinates (Å)		
Atom	X	Y	Z
C	2.385087	-1.252411	-0.14649
F	3.013005	-2.413250	-0.293315
C	1.001757	-1.193871	-0.125124
F	0.381477	-2.376419	-0.245001
C	0.282965	-0.019834	0.024456
F	-1.622000	1.050728	1.349179
C	1.063010	1.118928	0.163837
F	0.498667	2.319715	0.318355
C	2.446468	1.107822	0.150668
F	3.137362	2.232872	0.288824
C	3.115331	-0.090057	-0.008344
F	4.438620	-0.122383	-0.026130
C	-1.966398	-1.223256	-1.732359
C	-1.91105	-1.435302	1.132577
C	-1.804592	1.493290	-1.204879
H	-1.481045	-2.149082	-1.472102
H	-1.548667	-0.693579	-2.576305
C	-3.297958	-1.040601	-1.394684
H	-1.906339	-2.354462	0.556765
C	-3.142919	-1.349181	2.018124
H	-1.013249	-1.424696	1.750483
H	-0.809627	1.660736	-1.615989
C	-2.373624	2.764359	-0.593910

H	-2.444872	1.175411	-2.019982
H	-3.238733	0.076285	-0.082621
H	-3.81518	-1.769962	-0.785566
H	-3.937105	-0.350375	-1.927100
H	-4.067002	-1.407285	1.444205
H	-3.155871	-0.423571	2.589851
H	-3.140870	-2.182825	2.721318
H	-1.724059	3.184477	0.167073
H	-3.348847	2.575869	-0.144302
H	-2.506217	3.507834	-1.381239
P	-1.688679	0.072482	0.031014

TS-I.2 (PFP)

	Coordinates (Å)		
Atom	X	Y	Z
C	2.384815	-1.174506	-0.139737
F	3.039300	-2.317973	-0.288369
C	1.000342	-1.188218	-0.124447
F	0.404130	-2.381007	-0.245121
C	0.272748	-0.019971	0.026123
F	-1.628277	1.049662	1.345593
C	1.060065	1.112884	0.163068
F	0.519721	2.322413	0.318782
C	2.441466	1.031747	0.137586
F	3.156638	2.139378	0.272234
C	-1.964358	-1.219668	-1.724480
C	-1.915433	-1.433564	1.134708
C	-1.808959	1.494111	-1.204503
H	-1.477653	-2.144938	-1.463816
H	-1.548108	-0.691343	-2.570125
C	-3.300182	-1.044365	-1.395143
H	-1.900568	-2.355105	0.562593
C	-3.149404	-1.355207	2.018321
H	-1.019011	-1.412115	1.754764
H	-0.812588	1.654559	-1.615589
C	-2.367483	2.769491	-0.592948
H	-2.451178	1.180852	-2.020203
H	-3.252230	0.074645	-0.086237
H	-3.816542	-1.775160	-0.786984
H	-3.939476	-0.358047	-1.932426
H	-4.072055	-1.423919	1.443245
H	-3.171290	-0.427545	2.586465
H	-3.141029	-2.186008	2.724608
H	-1.713900	3.184151	0.167519
H	-3.344080	2.589329	-0.143063
H	-2.493808	3.513702	-1.380496

P	-1.706745	0.070864	0.028622
N	3.095357	-0.088341	-0.013127

Int I.B (HFB)

	Coordinates (Å)		
Atom	X	Y	Z
F	2.833728	-2.248231	0.583446
C	2.176964	-1.135880	0.292026
C	0.793053	-1.120319	0.267596
F	0.175529	-2.264742	0.533000
C	0.074910	0.022195	-0.053441
P	-1.763704	0.060848	-0.157015
C	0.813088	1.157036	-0.351622
F	0.194233	2.292404	-0.670281
C	2.194985	1.178024	-0.317421
F	2.863188	2.289079	-0.587170
C	2.879420	0.020321	0.004907
F	4.199924	0.017898	0.034004
C	-2.682299	-1.390000	-0.778258
F	-1.768770	-0.648233	1.395226
H	-3.548591	-1.479441	-0.122106
H	-2.063365	-2.262369	-0.574398
C	-3.082371	-1.299495	-2.241747
H	-3.684558	-0.411515	-2.432441
H	-3.666755	-2.171268	-2.530900
H	-2.205849	-1.249277	-2.885674
C	-2.723297	1.507830	0.415035
C	-3.303869	1.491092	1.820605
H	-3.509247	1.590434	-0.340491
H	-2.076950	2.371083	0.255681
H	-3.943027	0.624580	1.972593
H	-3.897375	2.389928	1.982794
H	-2.517154	1.454809	2.568822
H	-1.643169	0.659545	-1.462165

Int I.B (PFP)

	Coordinates (Å)		
Atom	X	Y	Z
F	2.878207	-2.171583	0.496152
C	2.197709	-1.067526	0.241526
C	0.812850	-1.120524	0.232154
F	0.215233	-2.280531	0.469691
C	0.087933	0.025787	-0.048071
P	-1.756107	0.055815	-0.160234

C	0.832003	1.165343	-0.302793
F	0.234631	2.319104	-0.589686
C	2.213870	1.114796	-0.251087
F	2.907144	2.216876	-0.479386
C	-2.680330	-1.400106	-0.755324
F	-1.740646	-0.624442	1.401347
H	-3.517882	-1.506457	-0.065695
H	-2.042988	-2.266989	-0.586458
C	-3.138341	-1.297933	-2.201207
H	-3.743221	-0.405841	-2.362207
H	-3.739235	-2.164619	-2.470483
H	-2.288858	-1.249230	-2.880073
C	-2.719154	1.509771	0.380532
C	-3.333306	1.491472	1.772010
H	-3.486031	1.594654	-0.393727
H	-2.065402	2.370322	0.238234
H	-3.973312	0.622919	1.909090
H	-3.934210	2.387980	1.917618
H	-2.565089	1.459535	2.539140
H	-1.615616	0.627393	-1.476262
N	2.878895	0.022454	0.011802

TS-I.3 (HFB)

	Coordinates (Å)		
Atom	X	Y	Z
C	2.279229	-1.198988	-0.005414
F	2.965884	-2.337995	0.077737
C	0.913057	-1.252342	-0.029456
F	0.302898	-2.454365	0.085242
C	0.078666	-0.097577	-0.269946
F	-2.119229	0.089113	1.556508
C	0.836808	1.119907	-0.079519
F	0.141407	2.271567	0.090800
C	2.204353	1.163250	-0.051085
F	2.811624	2.347854	0.019314
C	2.968233	0.006353	-0.050804
F	4.307752	0.045213	-0.128715
P	-1.662693	-0.094853	0.039276
C	-2.419846	-1.694480	-0.299180
C	-2.443038	1.315642	-0.780273
H	-1.997908	-2.116687	-1.206091
C	-3.942122	-1.576456	-0.386070
H	-2.134686	-2.332806	0.536241
H	-1.667991	1.817598	-1.353273
C	-3.129149	2.277940	0.187927
H	-3.155608	0.910851	-1.498008

H	-4.257366	-1.041912	-1.279582
H	-4.359642	-1.076610	0.487443
H	-4.369631	-2.575826	-0.429570
H	-2.418058	2.692417	0.898685
H	-3.925792	1.787885	0.743736
H	-3.563519	3.097548	-0.381080
H	-0.539543	-0.187730	-1.427478

TS-I.3 (PFP)

	Coordinates (Å)		
Atom	X	Y	Z
C	2.287635	-1.161675	-0.040790
F	2.986841	-2.293317	0.019661
C	0.930055	-1.255675	-0.023147
F	0.325068	-2.459001	0.032001
C	0.107424	-0.087708	-0.191604
F	-2.092064	0.114189	1.520174
C	0.897460	1.107164	-0.058781
F	0.259051	2.292781	0.041688
C	2.258596	1.052536	-0.067998
F	2.924668	2.204156	-0.014797
P	-1.629311	-0.073671	0.000064
C	-2.419893	-1.660529	-0.322983
C	-2.403768	1.347532	-0.805547
H	-2.087180	-2.052448	-1.279219
C	-3.942259	-1.511523	-0.270405
H	-2.078796	-2.334169	0.461288
H	-1.607878	1.939626	-1.248983
C	-3.270207	2.188524	0.128581
H	-2.989738	0.943073	-1.630651
H	-4.320327	-0.874204	-1.067771
H	-4.270447	-1.108605	0.686387
H	-4.394302	-2.493784	-0.390264
H	-2.676373	2.618670	0.931685
H	-4.072017	1.601647	0.572310
H	-3.716655	3.000747	-0.441736
H	-0.576890	-0.173373	-1.414828
N	2.986573	-0.044406	-0.089564

Table S10. Optimized geometries in Cartesian Coordinates (Å) of the intermediates and transition states of Mechanism II. M062X/6-311++G(3df,3pd). TS-II.1 ant Int II.A for HFB and PFP are not included since they are the same as TS-I.1 and Int I.A, respectively.

TS-II.1 (PFB)

	Coordinates (Å)		
Atom	X	Y	Z
F	0.650134	0.641103	2.225858
C	0.076284	0.519691	1.011749
C	-1.209111	0.056679	0.904887
F	-1.884473	-0.168941	2.036716
C	0.249959	0.528371	-1.351262
C	0.929574	0.715394	-0.112233
P	2.546905	-0.687172	0.028193
F	1.744836	1.854870	-0.056887
F	-1.555415	-0.122243	-2.650425
F	0.957794	0.736775	-2.478869
C	3.131490	-1.136743	-1.646704
C	1.660633	-2.116262	0.719550
H	3.244025	-0.200779	-2.191609
H	2.307439	-1.671178	-2.122829
C	4.433291	-1.937417	-1.706589
H	1.384525	-1.830326	1.736382
C	2.387669	-3.457599	0.702736
H	0.724794	-2.170219	0.156653
H	5.269311	-1.349283	-1.333109
H	4.650781	-2.200905	-2.740125
H	4.383701	-2.856687	-1.128078
H	3.358119	-3.396975	1.194520
H	2.540098	-3.809249	-0.315555
H	1.796256	-4.206092	1.226604
C	4.044778	-0.405905	1.034090
H	4.639399	-1.321852	1.024888
C	3.733662	0.036030	2.461989
H	4.619503	0.357699	0.507863
H	3.137413	-0.708457	2.987814
H	3.180451	0.972247	2.468381
H	4.659569	0.176110	3.015992
C	-1.040440	0.067530	-1.431309
C	-1.822097	-0.184416	-0.314946
H	-2.845596	-0.508928	-0.391151

TS-II.1 (PFT)

	Coordinates (Å)		
Atom	X	Y	Z
F	0.581529	0.723815	2.146503
C	0.042198	0.544788	0.926761
C	-1.217014	0.022252	0.806485
F	-1.893993	-0.205783	1.929125
C	-1.800521	-0.275677	-0.428169
C	-0.993338	-0.006843	-1.536878
C	0.268821	0.516524	-1.432376
C	0.909971	0.746079	-0.182250
P	2.558169	-0.676581	0.011736
F	1.707062	1.880318	-0.126794
F	-1.458381	-0.237918	-2.761858
F	0.992625	0.744318	-2.542875
C	3.170371	-1.145255	-1.649593
C	1.646597	-2.097153	0.691392
H	3.292413	-0.216030	-2.204174
H	2.353675	-1.685131	-2.132450
C	4.471634	-1.948274	-1.681409
H	1.338967	-1.800213	1.696107
C	2.370365	-3.440299	0.712862
H	0.728482	-2.157468	0.100451
H	5.302382	-1.358513	-1.298721
H	4.706033	-2.221104	-2.708832
H	4.410203	-2.862452	-1.095923
H	3.324572	-3.375784	1.235006
H	2.554660	-3.803354	-0.296144
H	1.760695	-4.181925	1.225456
C	4.037959	-0.412306	1.050204
H	4.628097	-1.331017	1.049481
C	3.693566	0.021567	2.473064
H	4.629181	0.351840	0.543465
H	3.091275	-0.729429	2.982603
H	3.134294	0.954485	2.472258
H	4.605669	0.165270	3.048567
S	-3.401176	-0.979148	-0.572187
H	-4.109739	0.152309	-0.709150

Int II.A (PFB)

	Coordinates (Å)		
Atom	X	Y	Z
F	-1.802660	-1.500456	3.078520
C	-2.043546	-0.909131	1.897913
C	-3.389547	-0.801123	1.569297

F	-4.294595	-1.267475	2.43153
C	-3.801289	-0.233387	0.387323
C	-2.814259	0.220229	-0.462763
C	-1.484031	0.100735	-0.118264
C	-1.026003	-0.454699	1.071904
F	-3.139984	0.776109	-1.630427
F	-0.588406	0.553133	-1.014909
C	1.097991	1.355125	1.150795
C	1.153025	-1.585623	-0.188929
H	0.13226	1.794314	0.928117
H	1.767870	1.556054	0.31471
C	1.663790	1.956250	2.437081
H	1.626159	-2.479938	0.219925
C	2.022157	-1.024797	-1.312998
H	0.174963	-1.871585	-0.562110
H	1.004303	1.773698	3.285567
H	1.758075	3.035003	2.319890
H	2.646039	1.551074	2.666057
H	1.619525	-0.095326	-1.710605
H	2.054161	-1.744964	-2.130088
H	3.037958	-0.848436	-0.97257
C	0.966053	-1.163636	2.953433
H	1.901320	-0.862277	3.415786
C	0.855352	-2.687532	2.937443
H	0.151265	-0.715509	3.510043
H	0.009114	-3.030601	2.342593
H	0.719353	-3.060481	3.951124
H	1.762787	-3.134415	2.533596
P	0.979618	-0.471323	1.266960
F	2.718162	-0.499328	1.336995
H	-4.847500	-0.151314	0.134578

Int II.A (PFT)

	Coordinates (Å)		
Atom	X	Y	Z
F	-1.8562	-1.366054	3.059356
C	-2.061034	-0.78358	1.868224
C	-3.400097	-0.634892	1.533424
F	-4.325396	-1.058342	2.398584
C	-3.794430	-0.067593	0.336981
C	-2.772107	0.336219	-0.507914
C	-1.452569	0.173795	-0.149523
C	-1.017218	-0.379988	1.049562
F	-3.079110	0.885750	-1.683437
F	-0.541130	0.585742	-1.047860
C	1.163719	1.358467	1.131278

C	1.136045	-1.587549	-0.188904
H	0.219781	1.827556	0.878313
H	1.863723	1.529961	0.313688
C	1.712549	1.950116	2.429329
H	1.578082	-2.493792	0.22826
C	2.032264	-1.057639	-1.306685
H	0.153319	-1.845471	-0.570097
H	1.021176	1.799694	3.258550
H	1.851004	3.023486	2.306963
H	2.671602	1.510489	2.691254
H	1.661341	-0.118307	-1.712064
H	2.050925	-1.781884	-2.120555
H	3.049502	-0.90982	-0.956994
C	0.928548	-1.147924	2.948605
H	1.872041	-0.886282	3.418125
C	0.751382	-2.665574	2.934323
H	0.129377	-0.663626	3.497589
H	-0.104013	-2.971874	2.332512
H	0.590543	-3.030308	3.94736
H	1.641573	-3.152860	2.538900
P	0.983107	-0.461834	1.260096
F	2.719276	-0.545422	1.350176
S	-5.462529	0.154927	-0.156381
H	-5.987953	-0.351452	0.964446

TS-II.2 (HFB)

	Coordinates (Å)		
Atom	X	Y	Z
F	-2.035245	-1.461812	2.976068
C	-2.258885	-0.893639	1.762181
C	-3.377155	-1.361202	1.091676
F	-4.172135	-2.300501	1.605526
C	-3.675845	-0.825624	-0.148292
C	-2.863983	0.163419	-0.674690
C	-1.765814	0.576867	0.059640
C	-1.397109	0.063404	1.280303
F	-3.163223	0.689584	-1.862976
F	-1.017790	1.552273	-0.522991
C	1.665232	1.132274	1.091773
C	0.745508	-1.606632	-0.078799
H	0.718036	1.654917	1.095297
H	2.110467	1.232056	0.098772
C	2.606308	1.662988	2.175802
H	1.290146	-2.550014	0.001896
C	1.012995	-0.944886	-1.429394
H	-0.309074	-1.809204	0.066514

H	2.139949	1.594684	3.155782
H	2.802976	2.714461	1.976362
H	3.558237	1.135729	2.183048
H	0.474534	-0.004295	-1.525482
H	0.677303	-1.609631	-2.222553
H	2.075986	-0.757909	-1.578240
C	1.040158	-1.233926	2.950655
H	1.937164	-0.984418	3.522301
C	0.791162	-2.742059	2.951155
H	0.208209	-0.680207	3.368346
H	-0.094053	-2.997851	2.371815
H	0.623297	-3.073152	3.973636
H	1.645134	-3.290736	2.555179
H	-0.715431	1.198038	2.728694
O	-0.327290	1.715358	3.468365
H	-1.079906	2.028866	3.974690
P	1.388339	-0.631245	1.297741
F	2.910207	-1.107908	1.173083
F	-4.742951	-1.244981	-0.820496

TS-II.2 (PFB)

	Coordinates (Å)		
Atom	X	Y	Z
F	-2.038531	-1.445335	2.992100
C	-2.255645	-0.884480	1.771004
C	-3.349161	-1.367907	1.071470
C	-3.657063	-0.861018	-0.175703
C	-2.843774	0.140663	-0.668805
C	-1.764308	0.590217	0.072137
C	-1.403870	0.088989	1.301426
F	-3.108243	0.674250	-1.869988
F	-1.023521	1.579214	-0.502116
C	1.668106	1.131870	1.091811
C	0.712931	-1.594885	-0.073313
H	0.724560	1.661323	1.096263
H	2.111709	1.226223	0.097565
C	2.615616	1.656631	2.172943
H	1.246996	-2.544641	0.003042
C	0.978698	-0.934190	-1.424758
H	-0.343020	-1.785277	0.079246
H	2.148947	1.596747	3.153311
H	2.823470	2.705195	1.969465
H	3.561995	1.119332	2.181519
H	0.448973	0.011856	-1.515776
H	0.630707	-1.594417	-2.216435
H	2.042618	-0.757892	-1.580183

C	1.036281	-1.231782	2.953198
H	1.933990	-0.979623	3.522572
C	0.791021	-2.740525	2.953075
H	0.203360	-0.680877	3.372600
H	-0.097367	-2.996610	2.378573
H	0.629643	-3.073332	3.976057
H	1.643728	-3.286831	2.551126
H	-0.700791	1.205388	2.735813
O	-0.309276	1.722843	3.476192
H	-1.060692	2.031703	3.987045
P	1.377680	-0.628899	1.299219
F	2.894093	-1.119640	1.162012
F	-4.117917	-2.330094	1.600983
H	-4.508589	-1.219859	-0.733928

TS-II.2 (PFP)

	Coordinates (Å)		
Atom	X	Y	Z
F	-1.977723	-1.855532	2.521594
C	-2.285170	-1.009968	1.504611
C	-3.509615	-1.196474	0.888308
F	-4.332913	-2.157082	1.306802
C	-3.106118	0.478035	-0.521141
C	-1.871862	0.709979	0.062499
C	-1.392204	-0.038102	1.112709
F	-3.513948	1.225814	-1.545521
F	-1.132257	1.721436	-0.459687
C	1.715947	1.049081	1.061873
C	0.869440	-1.728971	0.000830
H	0.751922	1.535927	0.985749
H	2.204437	1.105124	0.085982
C	2.588695	1.678223	2.149671
H	1.507562	-2.615090	0.021733
C	0.952812	-1.025497	-1.352178
H	-0.145772	-2.035317	0.228149
H	2.075880	1.667872	3.108134
H	2.774935	2.716975	1.884654
H	3.549839	1.175592	2.240664
H	0.341657	-0.124619	-1.367042
H	0.588164	-1.696478	-2.126763
H	1.979192	-0.756290	-1.598727
C	1.061954	-1.239754	3.004901
H	1.838804	-0.807689	3.640192
C	1.052350	-2.765989	3.103355
H	0.111678	-0.807519	3.293413
H	0.260635	-3.195627	2.492955

H	0.864929	-3.051316	4.136169
H	2.006651	-3.196625	2.803161
H	-0.720887	1.104057	2.612726
O	-0.375628	1.638529	3.354489
H	-1.146244	2.067627	3.733278
P	1.485052	-0.706969	1.348820
F	3.014802	-1.152204	1.312022
N	-3.918589	-0.463092	-0.115503

TS-II.2 (PFT)

	Coordinates (Å)		
Atom	X	Y	Z
F	-2.056824	-1.403366	3.019641
C	-2.251557	-0.858110	1.790010
C	-3.313148	-1.378560	1.072296
F	-4.077394	-2.352215	1.584935
C	-3.610618	-0.898528	-0.195151
C	-2.804327	0.124650	-0.674476
C	-1.758836	0.606165	0.092704
C	-1.408745	0.129115	1.333789
F	-3.049145	0.642066	-1.887529
F	-1.033179	1.605337	-0.480050
C	1.646796	1.140948	1.091015
C	0.651744	-1.576162	-0.082920
H	0.714745	1.688861	1.121799
H	2.070451	1.235437	0.088124
C	2.627234	1.638911	2.155294
H	1.178564	-2.529977	-0.007880
C	0.923989	-0.918349	-1.434520
H	-0.405598	-1.760084	0.067982
H	2.182034	1.576744	3.145552
H	2.847058	2.686153	1.957445
H	3.564597	1.086473	2.137027
H	0.405503	0.033748	-1.526738
H	0.568389	-1.575263	-2.225679
H	1.989697	-0.753924	-1.590534
C	1.007072	-1.231938	2.945963
H	1.917717	-0.996606	3.501711
C	0.745153	-2.737828	2.934844
H	0.188828	-0.675453	3.385883
H	-0.152850	-2.979978	2.369134
H	0.593424	-3.078862	3.956608
H	1.586746	-3.289117	2.516647
H	-0.697102	1.238705	2.772403
O	-0.281837	1.742458	3.509117
H	-1.016520	2.059367	4.038973

P	1.329315	-0.617593	1.291207
F	2.840965	-1.123813	1.135640
S	-4.971512	-1.577226	-1.076413
H	-4.812929	-0.805159	-2.156319

TS-II.3 (HFB)

	Coordinates (Å)		
Atom	X	Y	Z
F	-2.237318	-2.002855	1.764368
C	-2.240050	-0.945393	0.904675
C	-2.892483	-1.161638	-0.296493
F	-3.500660	-2.316660	-0.580179
C	-2.898584	-0.144855	-1.234311
C	-2.259847	1.047795	-0.946327
C	-1.631653	1.184162	0.281098
C	-1.586323	0.211045	1.247947
F	-2.263584	2.025585	-1.855861
F	-1.005036	2.374014	0.481854
C	1.910277	0.970855	1.244298
C	1.057952	-1.947826	1.116711
H	0.865292	1.212747	1.410343
H	2.093392	0.977450	0.167374
C	2.835077	1.944503	1.973761
H	1.550063	-2.908934	1.281245
C	0.770384	-1.733967	-0.372151
H	0.151223	-1.919928	1.711308
H	2.608040	1.970237	3.037811
H	2.681657	2.944283	1.574283
H	3.885172	1.686230	1.840035
H	0.279732	-0.778028	-0.548653
H	0.099482	-2.519661	-0.714410
H	1.681179	-1.783331	-0.966966
C	2.876278	-0.974518	3.388716
H	3.931442	-0.708679	3.303745
C	2.711400	-2.416773	3.865495
H	2.393993	-0.272700	4.060298
H	1.659205	-2.686477	3.944982
H	3.164350	-2.524980	4.848423
H	3.200496	-3.120586	3.193222
H	-0.552114	0.125418	2.604172
O	0.202109	-0.040179	3.296296
H	-0.205782	-0.561160	3.993359
P	2.200693	-0.720641	1.743755
F	3.480469	-1.074615	0.871739
F	-3.515108	-0.312003	-2.402472

TS-II.3 (PFB)

	Coordinates (Å)		
Atom	X	Y	Z
F	-2.167422	-2.310129	1.315004
C	-2.223515	-1.099420	0.692578
C	-2.874015	-1.077392	-0.528707
F	-3.432072	-2.196370	-1.019669
C	-2.943867	0.092406	-1.260236
C	-2.341506	1.210523	-0.718225
C	-1.705723	1.133888	0.510024
C	-1.614080	-0.009195	1.265662
F	-2.374636	2.371369	-1.393009
F	-1.125731	2.286966	0.952724
C	1.860479	0.884757	1.201714
C	1.098424	-2.040005	1.196230
H	0.836820	1.102581	1.493914
H	1.901480	0.853222	0.110669
C	2.846126	1.906185	1.768279
H	1.593030	-2.988429	1.418360
C	0.793100	-1.917581	-0.299261
H	0.198509	-1.978177	1.801940
H	2.756583	1.978506	2.850806
H	2.621159	2.884348	1.349667
H	3.877212	1.660711	1.516072
H	0.314504	-0.967776	-0.530880
H	0.102595	-2.710928	-0.578986
H	1.694418	-2.021187	-0.901568
C	2.903103	-0.926530	3.391909
H	3.948717	-0.624203	3.306365
C	2.772854	-2.344838	3.943544
H	2.383927	-0.212075	4.021477
H	1.725295	-2.625451	4.033761
H	3.224228	-2.388143	4.932265
H	3.282975	-3.071586	3.312513
H	-0.638371	-0.170744	2.671371
O	0.084046	-0.316922	3.397086
H	-0.150841	0.273880	4.116516
P	2.236137	-0.775250	1.734432
F	3.511683	-1.120652	0.863500
H	-3.449528	0.131538	-2.213107

TS-II.3 (PFP)

	Coordinates (Å)		
Atom	X	Y	Z
F	-2.200717	-2.106575	1.590284
C	-2.243348	-0.977832	0.834327
C	-2.960053	-1.043475	-0.346408
F	-3.587199	-2.169385	-0.692114
C	-2.427319	1.060660	-0.838631
C	-1.696431	1.181476	0.330912
C	-1.568094	0.151375	1.232234
F	-2.511652	2.086693	-1.686628
F	-1.079761	2.370029	0.546976
C	1.952875	0.936500	1.204328
C	1.111248	-1.978312	1.122370
H	0.896964	1.159956	1.326773
H	2.177238	0.931649	0.135385
C	2.829171	1.939428	1.953171
H	1.597554	-2.940021	1.300844
C	0.830073	-1.780955	-0.369888
H	0.201370	-1.938041	1.711914
H	2.554324	1.983341	3.005116
H	2.679354	2.928265	1.526079
H	3.887949	1.694683	1.871215
H	0.358867	-0.818595	-0.561974
H	0.144066	-2.557792	-0.702093
H	1.740617	-1.855733	-0.962226
C	2.912934	-0.966067	3.391505
H	3.980438	-0.757235	3.302945
C	2.671499	-2.374550	3.931523
H	2.463284	-0.212530	4.029070
H	1.606856	-2.594462	3.994313
H	3.094252	-2.454219	4.930501
H	3.146155	-3.130490	3.307491
H	-0.509936	0.085002	2.587256
O	0.249442	-0.039495	3.276432
H	-0.143372	-0.523652	4.007583
P	2.253618	-0.744318	1.735068
F	3.537626	-1.107866	0.875529
N	-3.053341	-0.037196	-1.178159

TS-II.3 (PFT)

	Coordinates (Å)		
Atom	X	Y	Z
F	-2.259274	-2.035461	1.744024
C	-2.232566	-0.963110	0.902317
C	-2.831504	-1.154960	-0.328067
F	-3.418394	-2.321802	-0.635586
C	-2.822068	-0.144181	-1.277761
C	-2.192008	1.037975	-0.916778
C	-1.612756	1.170424	0.334216
C	-1.595501	0.188431	1.293927
F	-2.145944	2.052847	-1.795211
F	-1.008087	2.365723	0.570675
C	1.805238	1.026603	1.339895
C	1.039019	-1.943157	1.121107
H	0.850412	1.338749	1.747079
H	1.724217	1.027844	0.250737
C	2.945358	1.932978	1.809072
H	1.581448	-2.878429	1.280003
C	0.766007	-1.729009	-0.370366
H	0.123319	-1.975986	1.699629
H	2.996387	1.970933	2.895941
H	2.761406	2.942611	1.448991
H	3.909637	1.606957	1.422120
H	0.222453	-0.802318	-0.547071
H	0.148332	-2.549133	-0.731921
H	1.688139	-1.718935	-0.949141
C	2.832983	-0.943956	3.413897
H	3.886895	-0.680971	3.309155
C	2.673993	-2.386009	3.892165
H	2.363542	-0.244129	4.097210
H	1.623056	-2.658771	3.976759
H	3.132132	-2.493336	4.872822
H	3.161608	-3.088378	3.217410
H	-0.608039	0.041032	2.648590
O	0.135809	-0.170318	3.350688
H	-0.270895	-0.784223	3.968603
P	2.121218	-0.676063	1.785273
F	3.400979	-0.960209	0.882621
S	-3.586742	-0.417428	-2.839018
H	-3.374289	0.820537	-3.296598

Table S11. Optimized geometries in Cartesian Coordinates (Å) of the intermediates and transition states of Mechanism III. M062X/6-311++G(3df,3pd). TS-III.1 ant Int III.A are not included since they are the same as TS-II.1 and Int II.A for PFT, respectively.

TS-III.2 (PFT)

	Coordinates (Å)		
Atom	X	Y	Z
C	1.592411	-0.962560	3.538910
F	1.948528	-0.354763	4.674902
C	0.668205	-0.325452	2.731909
F	0.224192	0.876952	3.127864
C	0.194954	-0.890718	1.561522
C	0.705428	-2.141417	1.248018
F	0.313242	-2.759121	0.131554
C	1.652070	-2.771429	2.032477
F	2.118578	-3.947527	1.623442
C	2.139582	-2.202446	3.209441
S	3.414782	-2.917474	4.154730
P	4.919955	-0.037164	3.346228
C	4.112957	1.544404	3.771630
H	3.944032	1.517504	4.848483
H	3.123503	1.518790	3.312798
C	4.879447	2.799658	3.363019
H	4.295515	3.687716	3.598750
H	5.826023	2.874228	3.895662
H	5.087817	2.811914	2.293228
C	5.122549	-0.041959	1.531445
H	5.837735	0.730801	1.249476
H	5.568700	-1.004312	1.275925
C	6.604027	0.007323	4.071478
H	6.507207	0.543716	5.017018
H	6.851611	-1.023419	4.327241
C	7.711138	0.611295	3.208446
H	7.482857	1.630609	2.903342
H	8.645583	0.628211	3.766513
H	7.872878	0.019241	2.309649
H	4.214654	-1.445069	3.888128
C	3.798849	0.152344	0.792273
H	3.957952	0.081663	-0.282174
H	3.067654	-0.603722	1.076251
H	3.367645	1.131606	0.999366
P	-1.010418	-0.015277	0.487345
C	0.288630	1.283852	0.016515
C	-1.321256	-0.545229	-1.250308
C	-2.135798	1.174583	1.321987
H	1.108041	0.743704	-0.466692
H	0.696379	1.713832	0.933502
C	-0.204980	2.403337	-0.901482

H	-0.523646	-0.178749	-1.891768
C	-2.685201	-0.059192	-1.746013
H	-1.300057	-1.629509	-1.253156
H	-1.527755	2.028906	1.610360
C	-2.932721	0.657103	2.514657
H	-2.812647	1.523199	0.538108
H	-0.570410	2.017424	-1.852641
H	0.598095	3.104968	-1.126586
H	-1.014090	2.972825	-0.444682
H	-2.735473	1.028086	-1.797531
H	-3.477961	-0.410277	-1.088008
H	-2.875211	-0.448219	-2.745035
H	-2.282247	0.183859	3.247828
H	-3.673909	-0.072873	2.207705
H	-3.438143	1.491529	2.999689
F	-2.115111	-1.302909	0.917925

Ionic Pair III.1 (PFT)

	Coordinates (Å)		
Atom	X	Y	Z
C	1.036090	-2.440562	2.452740
F	1.207144	-2.498713	3.775172
C	0.402929	-1.325121	1.943884
F	-0.009330	-0.391807	2.818034
C	0.113504	-1.179085	0.593815
C	0.569608	-2.207198	-0.222849
F	0.347632	-2.154710	-1.540233
C	1.219516	-3.313847	0.275335
F	1.596434	-4.249378	-0.597730
C	1.454686	-3.516182	1.650013
S	2.115661	-4.964360	2.284728
P	-1.013120	0.125534	0.010979
C	0.174195	1.531433	0.382330
C	-1.189125	0.501460	-1.779975
C	-2.307213	0.636954	1.215205
H	1.071487	1.346209	-0.213017
H	0.473983	1.461381	1.428058
C	-0.362949	2.933434	0.087945
H	-0.378058	1.161327	-2.079034
C	-2.547154	1.132914	-2.092073
H	-1.090395	-0.437403	-2.312287
H	-1.824354	1.309059	1.920889
C	-3.050912	-0.464739	1.964420
H	-3.015409	1.236353	0.638737
H	-0.589123	3.068308	-0.969260
H	0.371038	3.690967	0.359867

H	-1.272321	3.146668	0.650128
H	-2.673320	2.094611	-1.595627
H	-3.353808	0.473037	-1.779293
H	-2.637386	1.298716	-3.164286
H	-2.353937	-1.146878	2.453485
H	-3.683341	-1.037593	1.293312
H	-3.670401	-0.018551	2.741724
F	-2.123167	-1.286869	-0.393131
H	-1.492350	-2.972168	1.109905
P	-1.909155	-4.205724	1.608200
C	-1.197673	-5.491710	0.561299
C	-3.706757	-4.185015	1.453809
C	-1.419193	-4.345460	3.339878
H	-0.145623	-5.568642	0.852197
H	-1.230051	-5.103410	-0.458144
C	-1.898163	-6.845937	0.666575
H	-4.092002	-5.138887	1.815402
H	-4.065265	-3.409478	2.133411
C	-4.132559	-3.902657	0.011417
H	-0.354450	-4.597989	3.338816
H	-1.519168	-3.344245	3.763642
C	-2.232235	-5.362965	4.140898
H	-1.418427	-7.546010	-0.013057
H	-1.821505	-7.257806	1.670364
H	-2.951273	-6.783769	0.395897
H	-5.216285	-3.834489	-0.047002
H	-3.699784	-2.966718	-0.340895
H	-3.810820	-4.701412	-0.655704
H	-2.130327	-6.367438	3.736320
H	-1.864414	-5.381319	5.163857
H	-3.289576	-5.105909	4.168000

TS-III.3 (PFT)

	Coordinates (Å)		
Atom	X	Y	Z
C	1.044845	-2.460488	2.473532
F	1.198370	-2.577442	3.792826
C	0.468004	-1.306714	2.000849
F	0.100322	-0.368792	2.890522
C	0.217370	-1.089452	0.648988
C	0.653448	-2.095736	-0.209708
F	0.501036	-1.964313	-1.527351
C	1.242689	-3.245249	0.257482
F	1.615248	-4.153261	-0.645056
C	1.444256	-3.514481	1.628299
S	2.067219	-4.991116	2.208280

P	-0.789323	0.300824	0.160010
C	0.323034	1.731869	0.379652
C	-1.258433	0.380296	-1.594922
C	-2.123002	0.670482	1.351920
H	1.188298	1.546428	-0.258361
H	0.675120	1.708721	1.411511
C	-0.319543	3.077642	0.044293
H	-0.487936	0.970535	-2.092578
C	-2.647966	0.982171	-1.795643
H	-1.244260	-0.632464	-1.971087
H	-1.629974	1.282297	2.107552
C	-2.891492	-0.463802	2.018602
H	-2.806250	1.329338	0.814779
H	-0.627684	3.122307	-0.999372
H	0.393172	3.882113	0.212618
H	-1.192518	3.273631	0.665540
H	-2.726484	1.998825	-1.411672
H	-3.388497	0.353263	-1.305837
H	-2.871009	1.010788	-2.860235
H	-2.209010	-1.195470	2.448453
H	-3.524188	-0.973552	1.301829
H	-3.491553	-0.047425	2.826847
F	-2.219884	-1.721834	-0.311017
H	-1.811363	-2.884290	0.709993
P	-2.049273	-4.143415	1.379570
C	-1.276013	-5.489838	0.450265
C	-3.849827	-4.312899	1.262596
C	-1.553897	-4.221327	3.128128
H	-0.200499	-5.405459	0.617537
H	-1.464120	-5.279649	-0.603417
C	-1.758529	-6.883544	0.846668
H	-4.159724	-5.236275	1.750980
H	-4.269254	-3.483517	1.835517
C	-4.304627	-4.253348	-0.196757
H	-0.527336	-4.597355	3.140194
H	-1.522662	-3.197172	3.500588
C	-2.466241	-5.079885	4.005432
H	-1.289940	-7.625600	0.204116
H	-1.476710	-7.114433	1.872406
H	-2.838876	-6.987141	0.748186
H	-5.391221	-4.246298	-0.249504
H	-3.916585	-3.352869	-0.672343
H	-3.949395	-5.121242	-0.751547
H	-2.540084	-6.101441	3.637571
H	-2.059889	-5.117820	5.013652
H	-3.471352	-4.665936	4.062623

Int III.B (PFT)

	Coordinates (Å)		
Atom	X	Y	Z
C	-2.305467	-1.011533	-0.837347
F	-2.883120	-2.030712	-1.467790
C	-0.968021	-1.108824	-0.574338
F	-0.325594	-2.225269	-0.945371
C	-0.249304	-0.096188	0.078547
C	-1.020133	1.002714	0.487291
F	-0.421085	1.993021	1.166235
C	-2.356756	1.107086	0.227327
F	-2.984247	2.198567	0.656242
C	-3.091228	0.108020	-0.462238
P	1.473765	-0.211761	0.434920
C	1.692669	-0.868018	2.107667
C	2.300743	-1.295824	-0.767178
C	2.259980	1.414349	0.342152
H	1.094518	-1.779655	2.146272
H	1.207915	-0.143759	2.765296
C	3.136455	-1.133155	2.530191
H	2.123016	-2.318730	-0.436644
C	3.794823	-1.016129	-0.941944
H	1.775034	-1.177216	-1.713111
H	1.926192	1.995212	1.198729
C	1.958926	2.130678	-0.974045
H	3.329358	1.236959	0.462485
H	3.578912	-1.933285	1.940525
H	3.156365	-1.440452	3.573129
H	3.758292	-0.244406	2.434135
H	4.340266	-1.058614	-0.002124
H	3.966993	-0.041027	-1.392417
H	4.216272	-1.766820	-1.606330
H	0.900866	2.369307	-1.052951
H	2.233189	1.521499	-1.834793
H	2.523286	3.058576	-1.023589
S	-4.739016	0.232154	-0.787207

TS-III.4 (PFT)

	Coordinates (Å)		
Atom	X	Y	Z
F	1.091549	1.653843	1.570739
C	0.402089	0.867375	0.762592
C	-0.861999	0.545855	1.068737
F	-1.396848	0.999595	2.190868
C	-1.703431	-0.248015	0.193672

C	-1.080651	-0.616027	-1.065245
C	0.183569	-0.297195	-1.361025
C	1.087688	0.426994	-0.461437
P	2.607170	-0.594609	-0.121485
F	-1.806750	-1.294996	-1.937853
F	0.714531	-0.702975	-2.510581
C	3.690656	-0.615073	-1.576001
C	1.927729	-2.255133	0.194549
H	4.486376	0.081866	-1.325483
H	3.127078	-0.134919	-2.372555
C	4.206255	-1.987135	-1.996288
H	1.156611	-2.092843	0.952378
C	2.928014	-3.322939	0.661668
H	1.407097	-2.582605	-0.705825
H	4.835119	-2.437467	-1.230609
H	4.810733	-1.868835	-2.893107
H	3.395697	-2.675017	-2.231773
H	3.761252	-2.902332	1.222251
H	3.340174	-3.868176	-0.181017
H	2.424684	-4.037982	1.308275
C	3.461777	-0.095662	1.392037
H	4.471458	-0.499486	1.283302
C	2.819726	-0.569811	2.695340
H	3.538453	0.986259	1.313955
H	1.783767	-0.251407	2.783802
H	3.364274	-0.136077	3.531117
H	2.851737	-1.651451	2.801617
S	-3.231908	-0.667128	0.574533
H	1.664015	1.304466	-0.892547
F	3.169016	1.825486	-0.679965

Ionic Pair III.2 (PFT)

	Coordinates (Å)		
Atom	X	Y	Z
S	-0.452683	-0.400147	1.606642
C	1.101959	-0.206879	0.819406
C	1.747240	1.028161	0.748190
F	1.200675	2.104378	1.309852
C	2.959210	1.181988	0.100327
F	3.515712	2.391810	0.057619
C	3.595687	0.111179	-0.492754
H	4.542119	0.233049	-0.996218
C	2.986164	-1.123498	-0.407136
F	3.568144	-2.190354	-0.953081
C	1.774236	-1.282451	0.238966
F	1.252766	-2.507096	0.289518

H	0.400947	0.325084	-1.825990
C	-0.418402	-0.203844	-2.311112
H	0.010379	-0.868783	-3.058412
H	-1.044530	0.523491	-2.826440
C	-1.234516	-1.024374	-1.308828
H	-2.023521	-1.564269	-1.829927
H	-0.618735	-1.738164	-0.776793
P	-2.108442	0.068634	-0.135030
F	-3.312446	0.316811	-1.258426
C	-3.298865	-0.616492	1.062360
H	-2.954729	-0.430038	2.075818
H	-4.225719	-0.068811	0.900464
C	-1.646838	1.832652	-0.034020
H	-1.710564	2.088434	1.022036
H	-0.587223	1.876943	-0.280690
C	-2.450879	2.794900	-0.901535
H	-2.357705	2.556359	-1.957792
H	-3.507252	2.773663	-0.647243
H	-2.077565	3.805138	-0.741738
C	-3.502520	-2.111835	0.815051
H	-2.567928	-2.655523	0.945392
H	-4.227230	-2.506259	1.523849
H	-3.879696	-2.294468	-0.189966

TS-III.5 (PFT)

	Coordinates (Å)		
Atom	X	Y	Z
C	-0.151766	-0.961748	-1.185554
C	1.089806	-0.564739	-0.733435
C	1.327485	0.739494	-0.347450
C	0.344501	1.726470	-0.412060
C	-0.907392	1.305319	-0.859335
C	-1.145099	-0.003986	-1.235102
H	-0.341145	-1.981108	-1.483129
S	0.664494	3.399775	-0.013359
H	2.014549	3.402569	-0.875288
O	3.032300	3.300293	-1.584519
H	3.511092	2.544228	-1.226235
P	2.952697	3.415527	-3.460905
C	2.110646	1.807433	-3.547593
C	4.770437	3.471368	-3.472546
C	1.942779	4.910056	-3.240313
H	1.680423	1.729468	-4.542197
H	1.299080	1.824578	-2.822131
C	3.045880	0.627059	-3.277395
H	5.094136	3.088424	-4.437131

H	5.160070	2.822891	-2.691709
C	5.260957	4.907462	-3.270024
H	2.372528	5.656789	-3.905945
H	2.011536	5.268012	-2.218505
C	0.486034	4.635643	-3.629647
H	3.469324	0.654023	-2.273440
H	2.489711	-0.304375	-3.363922
H	3.866296	0.597106	-3.993106
H	6.348251	4.930213	-3.269306
H	4.911972	5.554498	-4.073101
H	4.910348	5.309316	-2.320844
H	-0.080309	5.563190	-3.584702
H	0.417452	4.242838	-4.642321
H	0.022765	3.933308	-2.938058
F	2.909076	3.616958	-5.118563
F	2.561423	1.049017	0.076451
F	2.090628	-1.444711	-0.670742
F	-1.904754	2.179353	-0.957088
F	-2.361751	-0.335525	-1.664841

Table S12. Optimized geometries in Cartesian Coordinates (Å) of the intermediates and transition states of Mechanism III. M062X/6-311++G(3df,3pd).

Complex IV.1 (TFT)

	Coordinates (Å)		
Atom	X	Y	Z
C	-1.886062	0.564495	-1.964036
C	-1.878846	0.336049	-0.602671
C	-0.820544	0.743071	0.185795
C	0.278444	1.397447	-0.357205
C	0.263347	1.623173	-1.726896
C	-0.798752	1.214003	-2.510657
H	-2.712978	0.246007	-2.579108
F	1.287888	2.247662	-2.311014
F	-0.755546	1.460085	-3.817801
F	-2.902336	-0.286335	-0.025305
F	-0.851466	0.504106	1.494636
S	1.582595	1.880336	0.706533
H	2.358866	2.431895	-0.242344
O	3.830563	3.364755	-1.401625
H	3.423125	3.342836	-2.271163
H	4.058169	4.285348	-1.252471

TS-IV.1 (TFT)

	Coordinates (Å)		
Atom	X	Y	Z
C	-1.516135	0.458129	-2.111826
C	-1.225642	0.029931	-0.830269
C	-0.293320	0.704480	-0.059546
C	0.391015	1.813300	-0.497231
C	0.077029	2.214220	-1.772155
C	-0.845267	1.570790	-2.579719
H	-2.238798	-0.059019	-2.723956
F	0.700618	3.301269	-2.312013
F	-1.092688	2.020554	-3.819198
F	-1.854229	-1.048433	-0.339169
F	-0.074373	0.220015	1.186547
P	2.296665	4.732961	2.476876
C	4.036693	4.259194	2.735581
C	1.408917	4.672129	4.056303
C	2.261594	6.448843	1.878804
H	4.364054	3.802372	1.800551
H	4.017846	3.461426	3.479670
C	4.984418	5.388588	3.140042
H	0.369767	4.913819	3.827546
C	1.964497	5.582929	5.148660

H	1.424343	3.626366	4.366288
H	2.847663	7.066661	2.560572
C	0.837283	6.981154	1.733222
H	2.779343	6.446114	0.917818
H	5.075771	6.125498	2.344797
H	5.975073	4.980633	3.329562
H	4.653240	5.900887	4.040956
H	2.009500	6.621592	4.822523
H	2.963639	5.273193	5.448723
H	1.325076	5.537533	6.027656
H	0.347970	7.065219	2.702600
H	0.237731	6.328791	1.100888
H	0.855776	7.970623	1.282525
S	1.270967	3.325276	1.196263
H	2.236624	3.488767	0.286232
O	3.344946	2.476364	-1.269782
H	2.993183	2.913761	-2.050595
H	2.602535	1.925528	-0.978914

[1] Fitch, S. J. *J. Am. Chem. Soc.* **1964**, 86, 61.