Supporting Information For:

Sustainable Defluorination Pathway: From Perfluoro Gem-diol Hydration to Electrocatalytic Removal of CF_3 at Room Temperature

Contents

^{19}F,^{13}C NMR spectra, MS, FT-IR data

Fig S1 ^{13}C NMR (101 MHz,$CDCl_3$) of PF-2M3B

δ 175.7~176.7(-C=O),111.2~121.0(-CF_3),89.4~92.3(-CF-);

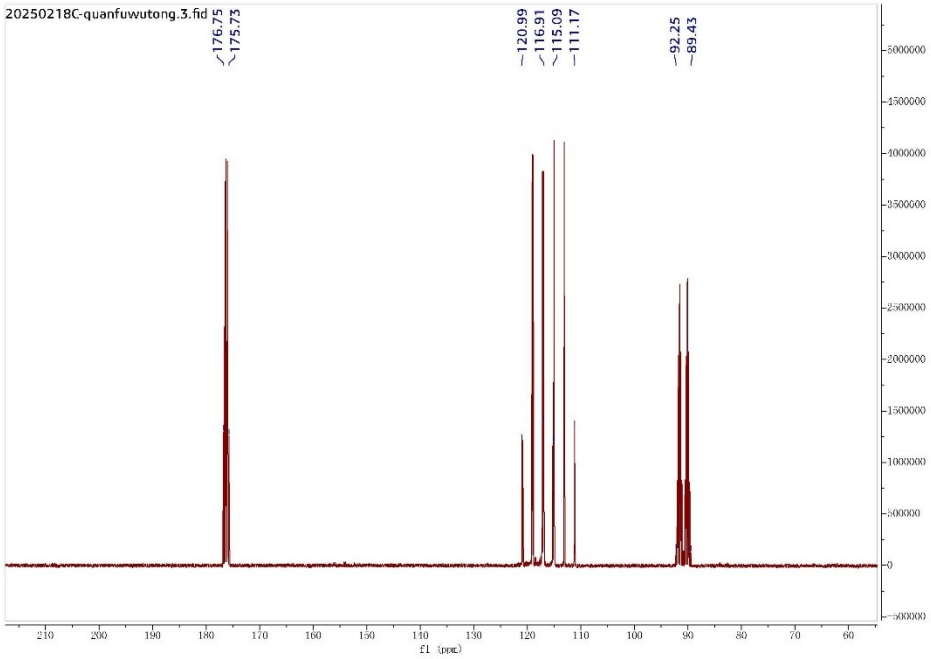


Fig S2 ^{19}F NMR (376 MHz,$CDCl_3$) of PF-2M3B

δ -76.7 (d, 6F),-78.5 (s,3F),-193.1 (s, 1F).

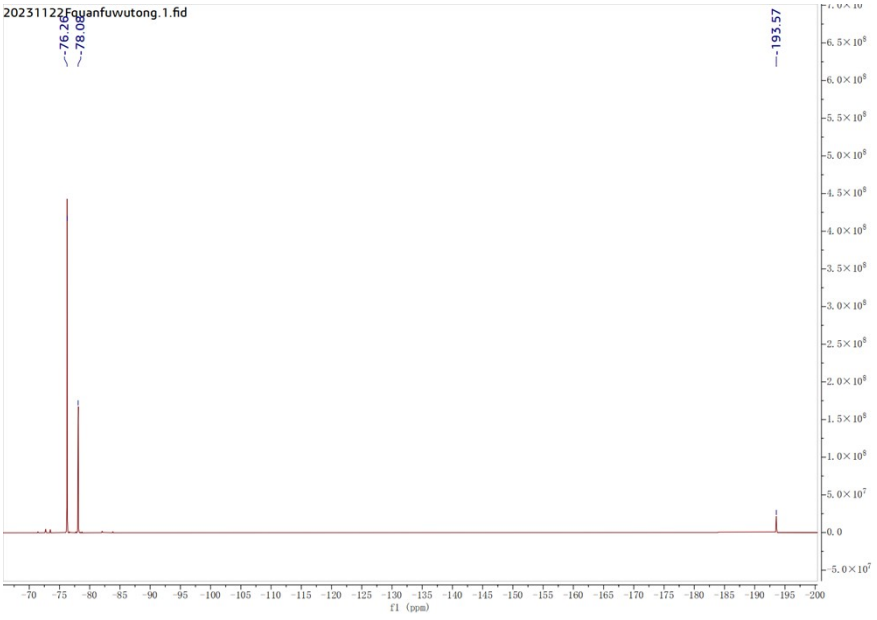


Fig S3 ^{13}C NMR (101 MHz,$CDCl_3$) of PF-2M3B gem-doil

δ 116.4~123.7(-CF_3), 92.9~93.6 (-CF-),89.6~92.6(-C(-OH)$_2$);

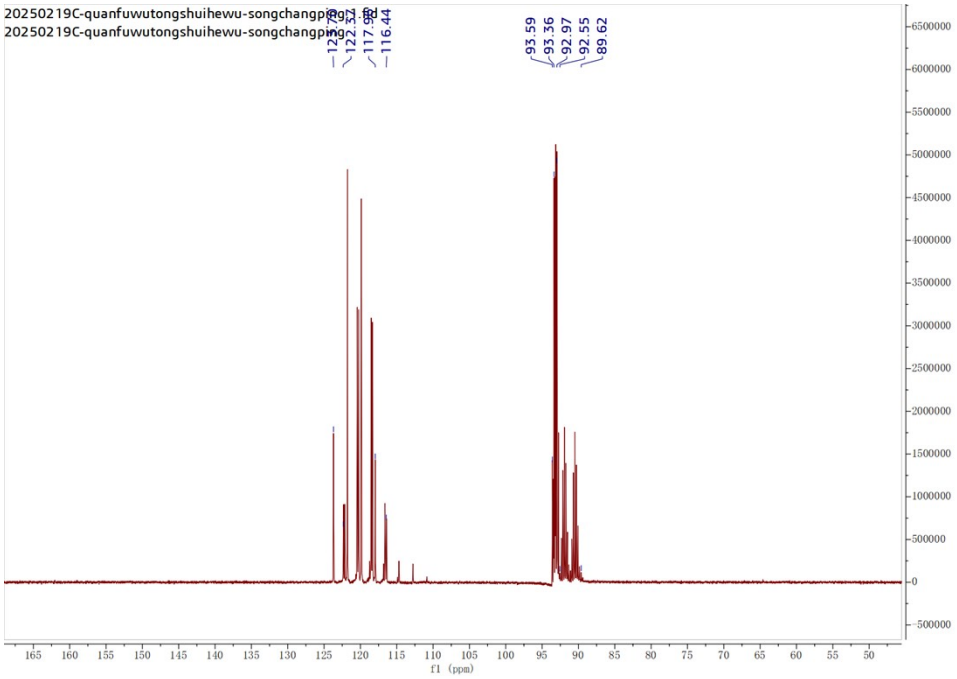
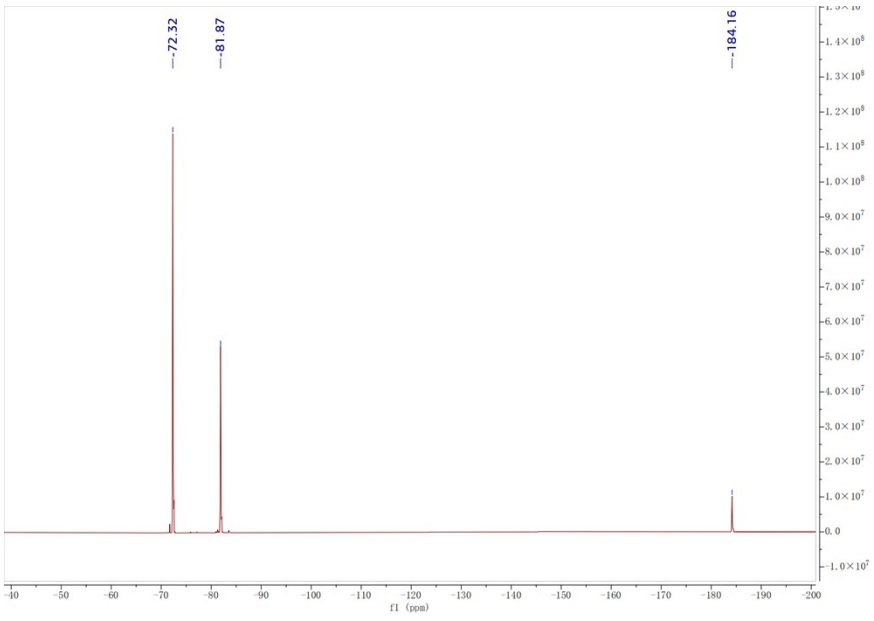


Fig S4 ^{19}F NMR (376 MHz,$CDCl_3$) of PF-2M3B gem-doil

^{19}F NMR (376 MHz, $CDCl_3$)　δ -72.6 (d, 6F),-81.9(s, 3F),-184.0 (s,1F)。



The comprehensive judgment based on the ^{13}C NMR and ^{19}F NMR indicates that PF-2M3B and PF-2M3B gem-diol are different, and it is not simply dissolved in water.

Fig S5 MS of PF-2M3B

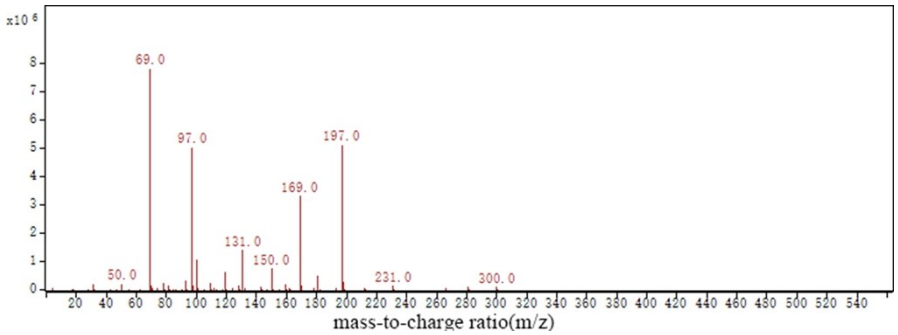
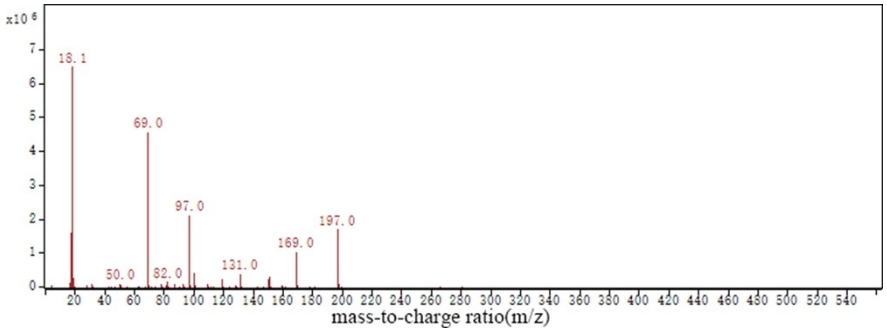


Fig S6 MS of PF-2M3B gem-doil



From MS, the sole difference between PF-2M3B and PF-2M3B gem-diol lies in whether there is bound water (m/z=18) or not, which also provides a clear indication for determining whether the product form is gem-diol or ketone.

Fig S7 FT-IR of PF-2M3B

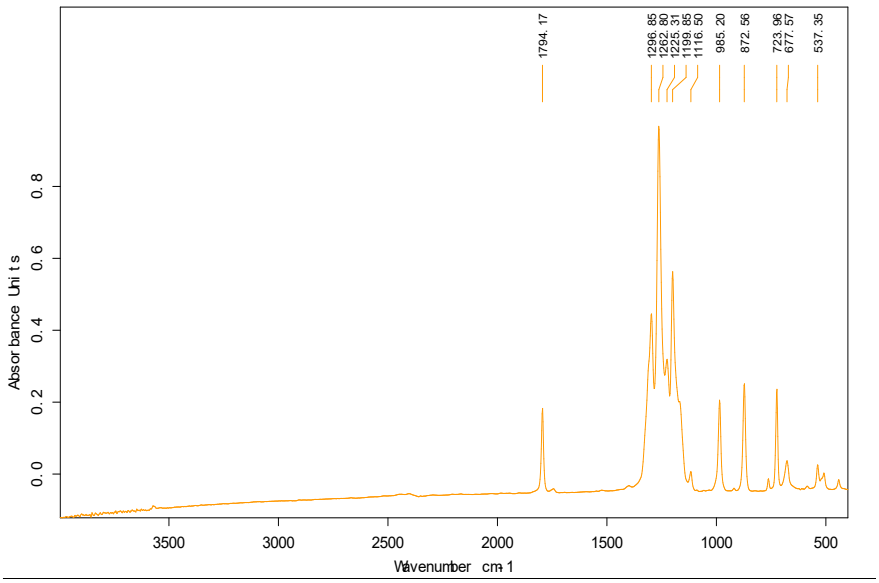
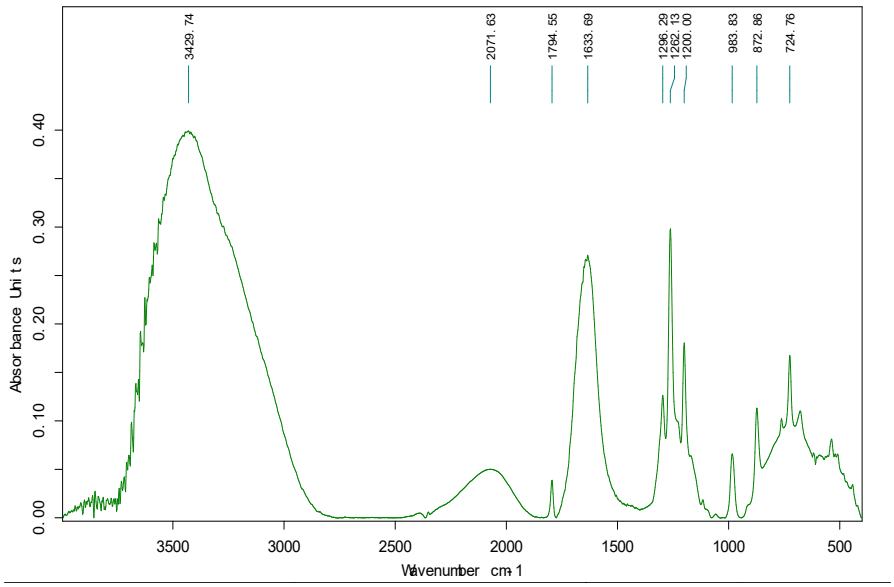
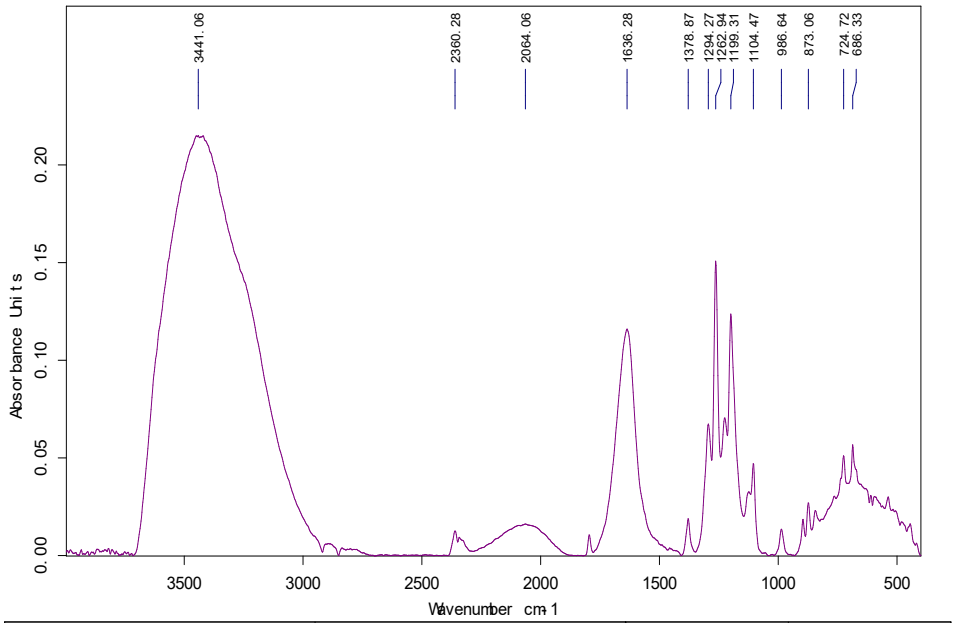


Fig S8 FT-IR of PF-2M3B gem-doil



FT-IR analysis reveals that in PF-2M3B gem-diol, the carbonyl absorption peak of PF-2M3B at 1794 cm^{-1} remains, suggesting that the glycol and ketone are reversible. Nevertheless, the gem-diol structure of this substance predominates at room temperature.

Fig S9 FT-IR of PF-2M3B gem-doil after the electrocatalytic reaction



By comparing the FT-IR spectra before and after the electrocatalytic reaction, it can be observed that a significant absorption peak at 1378 cm^{-1}. In combination with the notable change in the peak shape at 2900 cm^{-1}, it is concluded that the defluorination reaction has taken place to form the C-H bond structure.

Fig S10 FT-IR of PF-A gem-doil

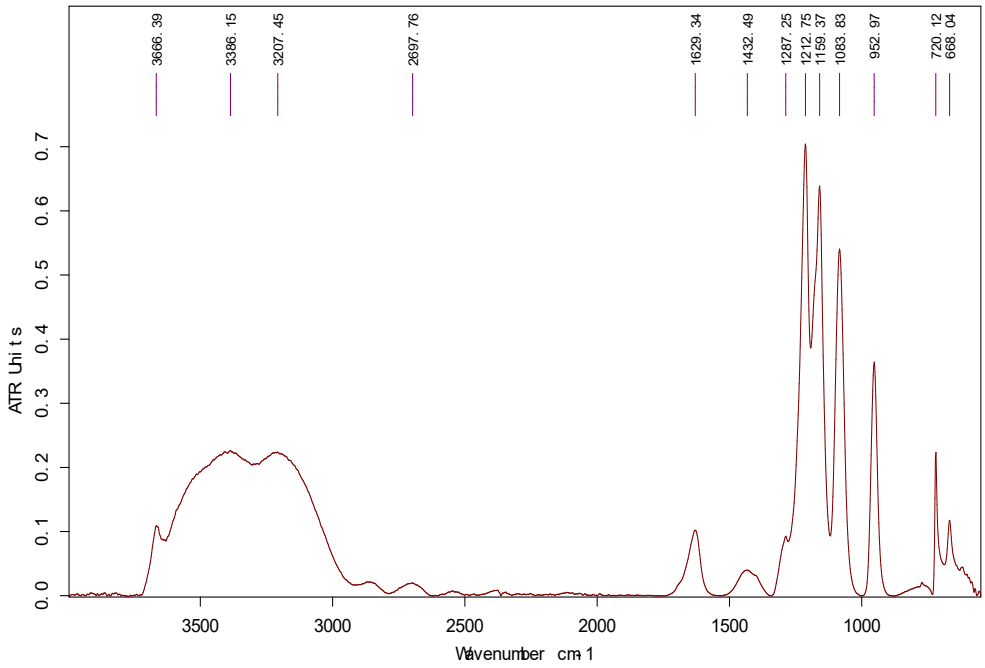
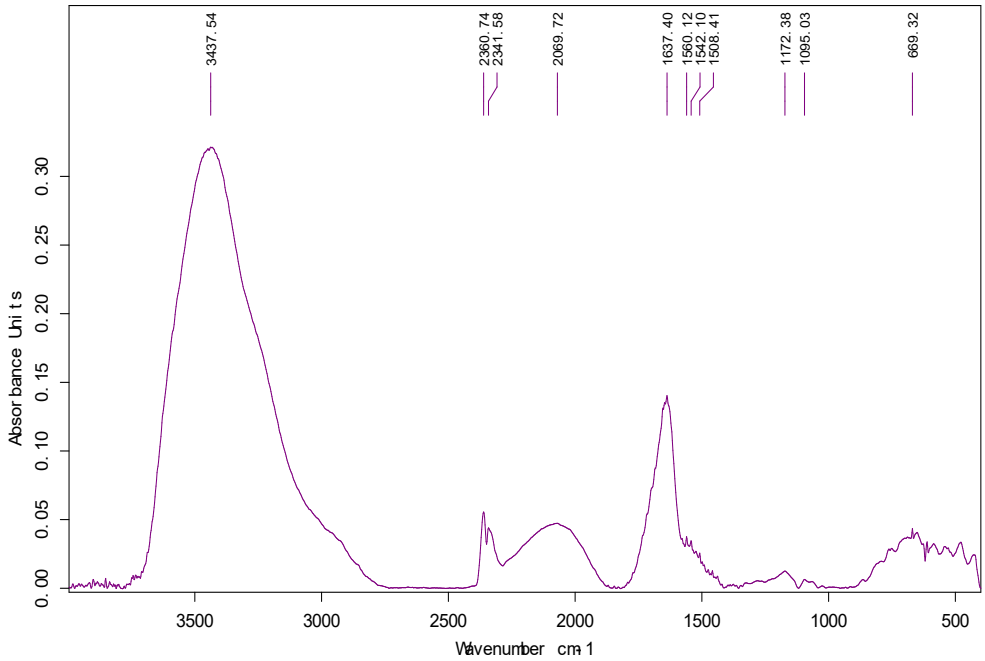
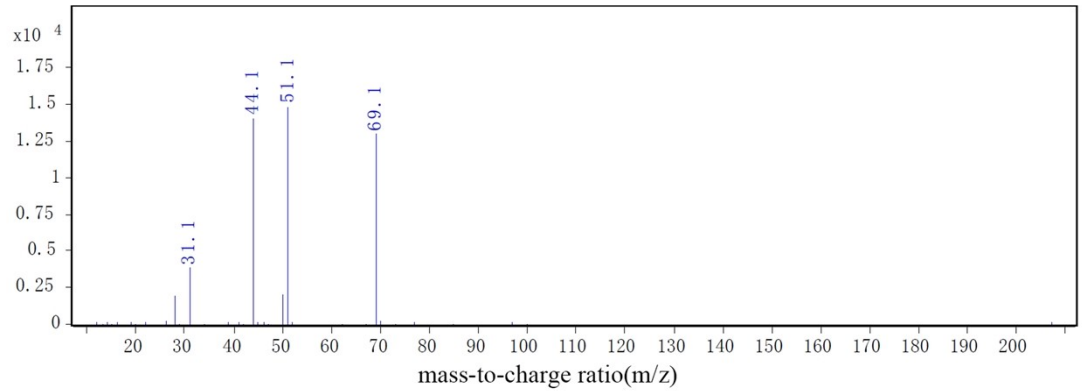


Fig S11 FT-IR of PF-A gem-doil after the electrocatalytic reaction



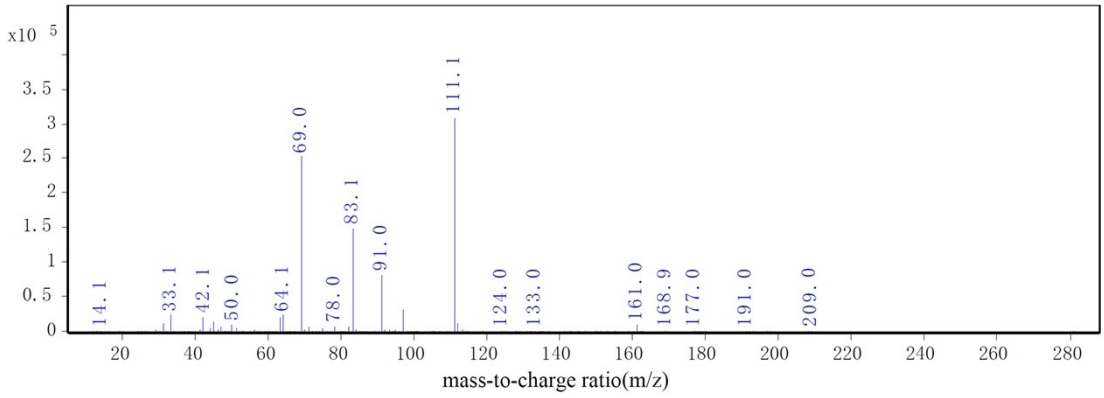
Unlike the electrocatalytic reaction of PF-2M3B gem-diol, the significance at 1378 cm^{-1} is not prominent, but the C-F bond within the range of 1000 - 1400 cm^{-1} is evidently weakened. Furthermore, the peaks at 2360, 2341 and 669 cm^{-1} in the FT-IR analysis are comprehensively regarded as dissolved CO2.

Fig S12 MS of CF3H in the system



MS analysis indicated that CF_3H was present in the solution after the electrocatalytic reaction, thereby confirming the removal of the CF_3. Additionally, along with CF_3H, CO_2 was also detected in the mass spectrum. The existence of dissolved CO_2 was verified by infrared spectroscopy.

Fig S13 MS of Fig.4 C1



The structures of Fig. 4 B1, B2 and Fig. 4 C2 were not detected. Therefore, the possible reaction paths have to be inferred based on theoretical calculations.

Fig S14 MS of Fig.4 D

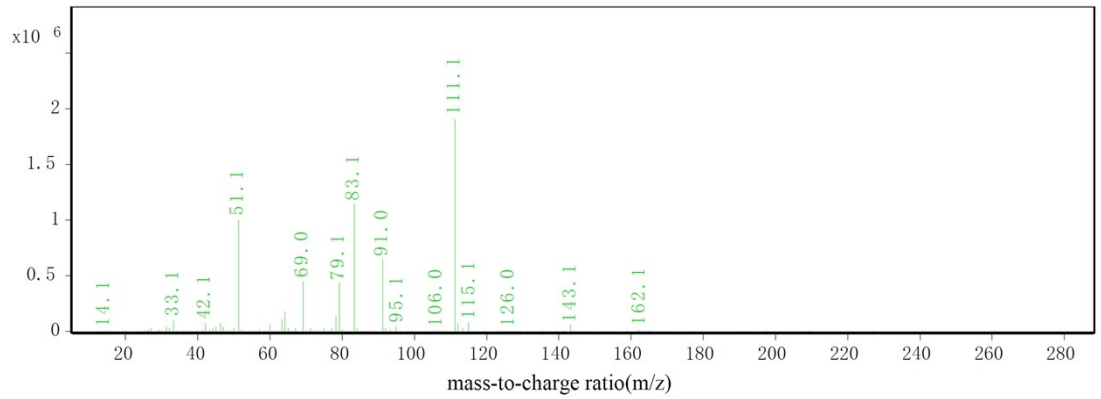


Fig S15 MS of Fig.4 E

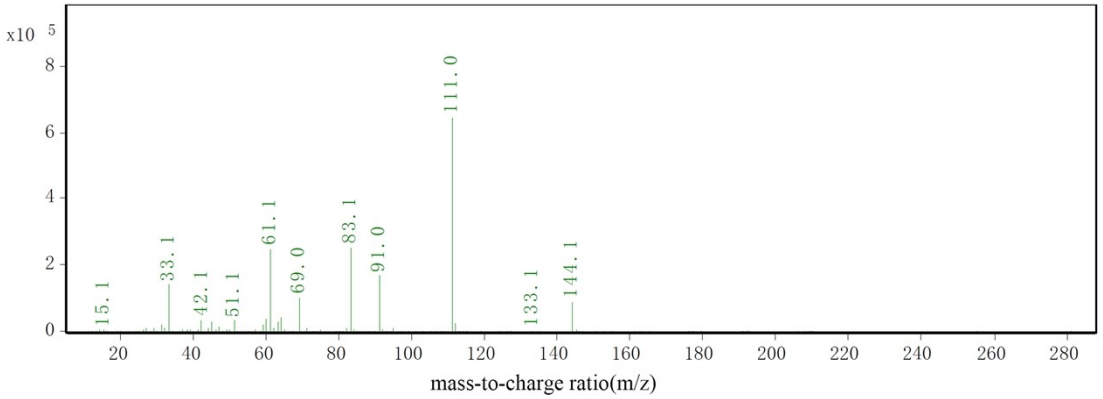


Fig S16 MS of Fig.4 F

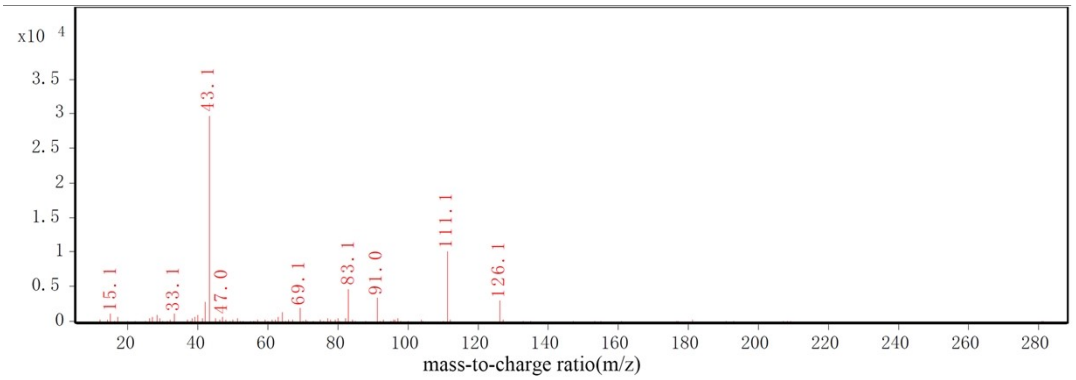
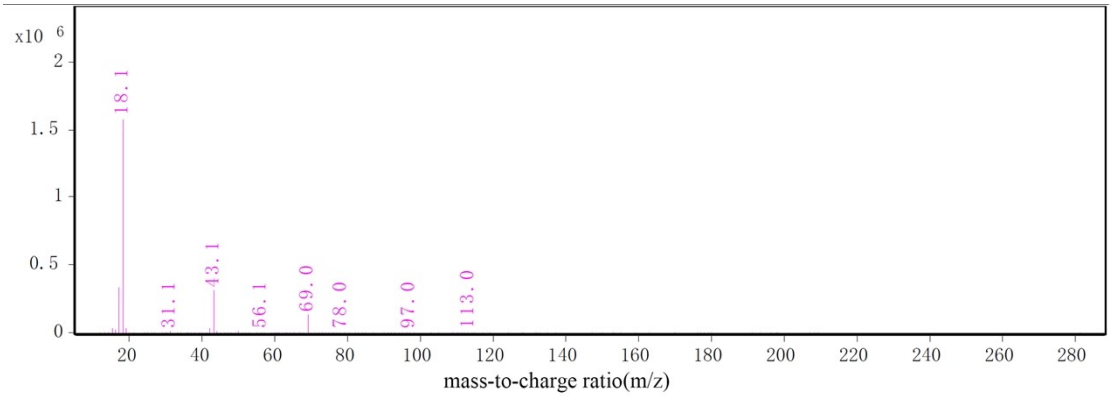


Fig S17 MS of Fig.5 D



The substances B and C in Fig. 5 were not detected. Based on the analysis of energy barriers, substances B and C are reactive and tend to be unstable.

The substances E1 and E2 in Fig. 5 were not detected. Nevertheless, as the substance D contains the peak of water, it is judged that a large amount of gem-diol structure can still stably exist at room temperature. Hence, theoretical calculations are supplemented.

Fig S18 MS of Fig.5 F

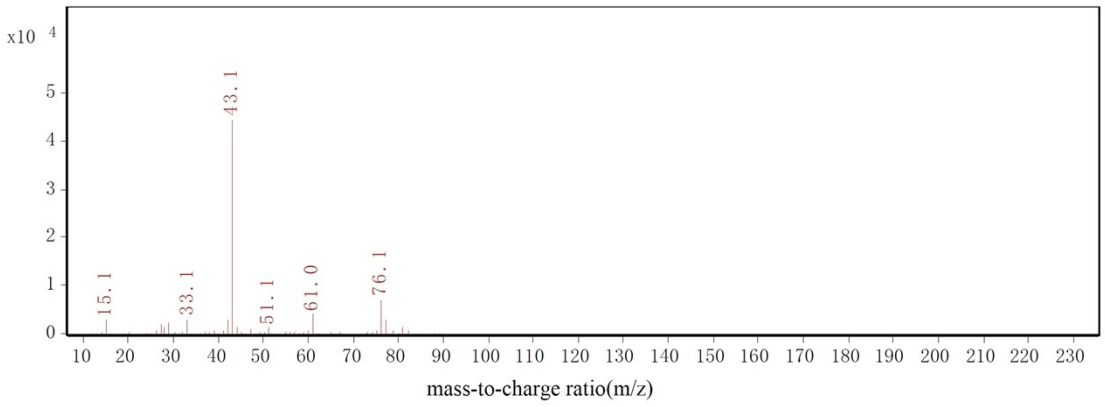


Fig S19 MS of Fig.5 G

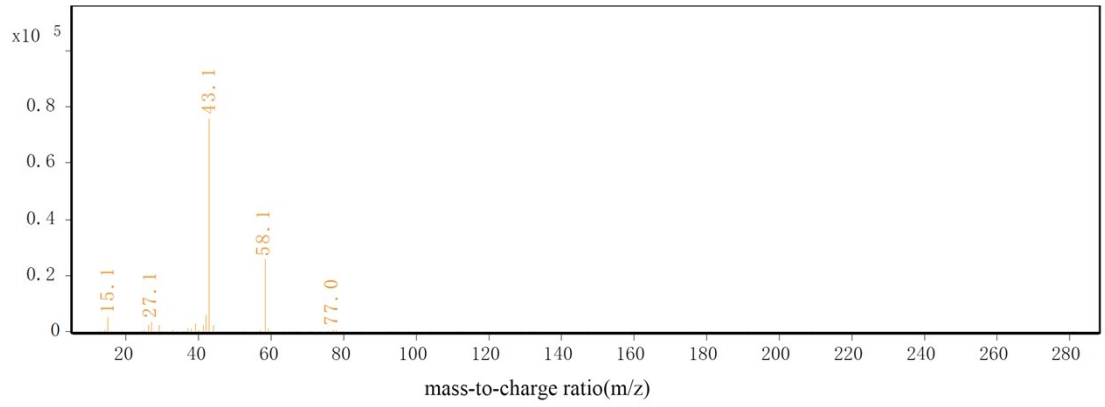


Fig S20 GC of the PF-A reaction for 24 hours (Zn)

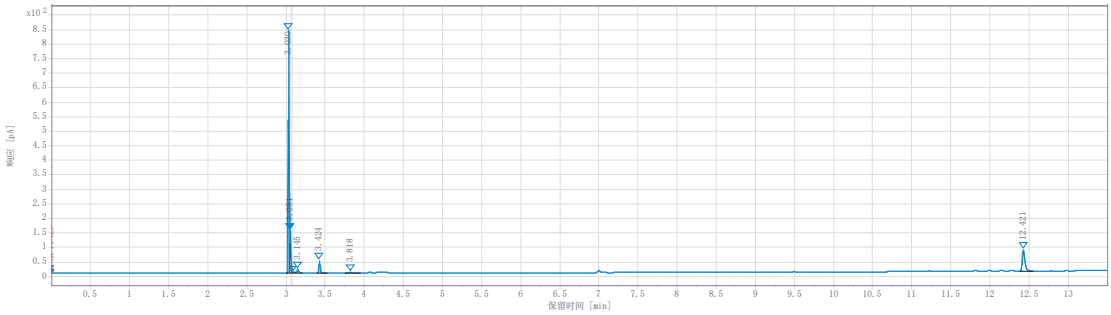
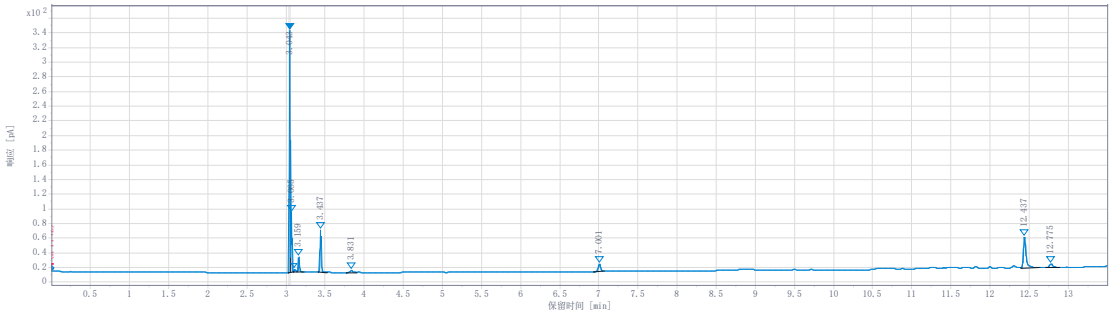


Fig S21 GC of the PF-A reaction for 48 hours (Zn)



The detection of CF_3H relies on Agilent 5977B GC/MSD. It cannot be reflected in the purity test (Agilent 7890B) and is expressed as detectable.

Compound	Time（min）	content /wt%	
		24h	48h
PF-A gem-diol	3.03	63.35	43.87
D	3.05	11.86	11.22
C	3.16	0.6	1.1
F	3.42	4.72	11.68
E2	3.83	1.49	3.85
EtOH	7.00	-	4.42
G	12.4	17.43	19.38
recombinant fraction	12.78	-	3.27
Other	-	0.55	4.48

Fig S22 GC of the PF-2M3B reaction for 24 hours (Pb/C)

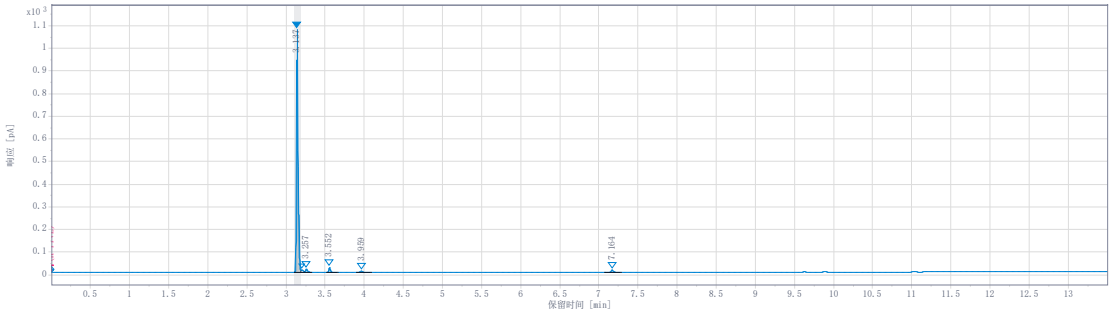
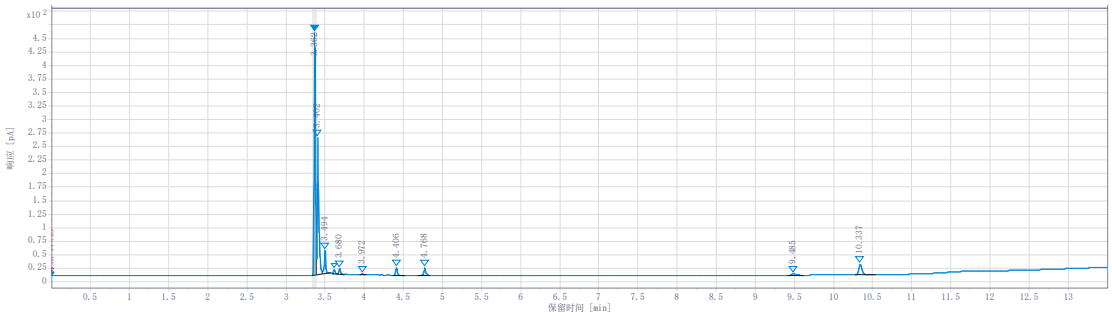
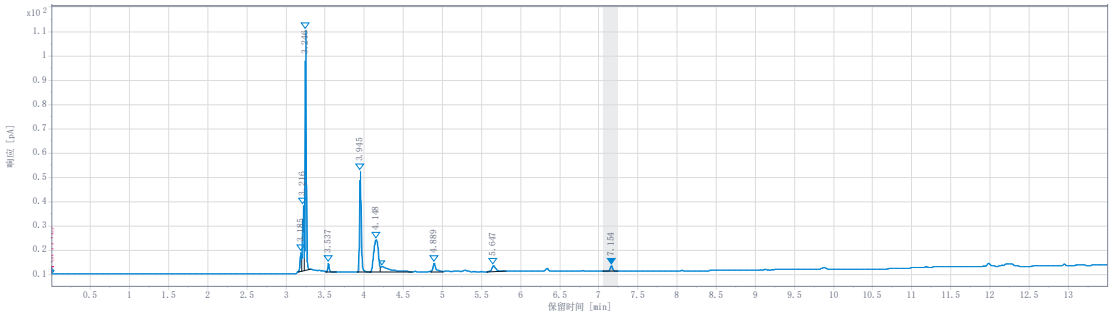


Fig S23 GC of the PF-2M3B reaction for 24 hours (Zn)



The operation error during the detection caused a time delay of about 0.15 minutes, but it didn't affect the relative displacement.

Fig S24 GC of the PF-2M3B reaction for 48 hours (Zn)



Compound	Time（min）	content /wt%		
		5%Pb/C 24h	**Zn 24h**	**Zn 48h**
PF-3M2B gem-diol	3.14	93.16	48.38(51.38)	13.83
C1	3.25	1.23	32.98(35.03)	31.29
D	3.54	1.47	5.11(5.43)	1.39
E	3.95	1.86	1.24(1.32)	20.01
F	4.15	0.79	2.04(2.17)	25.8
Unknown	4.8	-	2.21(2.35)	2.99
Butanone	5.65	-	-	2.98
EtOH	7.15	1.48	-	1.68
Other	-	0.01	2.20(2.35)	3.02
Filler loss	10.34	-	5.84	-

* Zn 24h: The content in parentheses is the percentage after excluding Filler loss

Fig S25 Mayer bond order analysis of defluorination in PF-A gem-diol

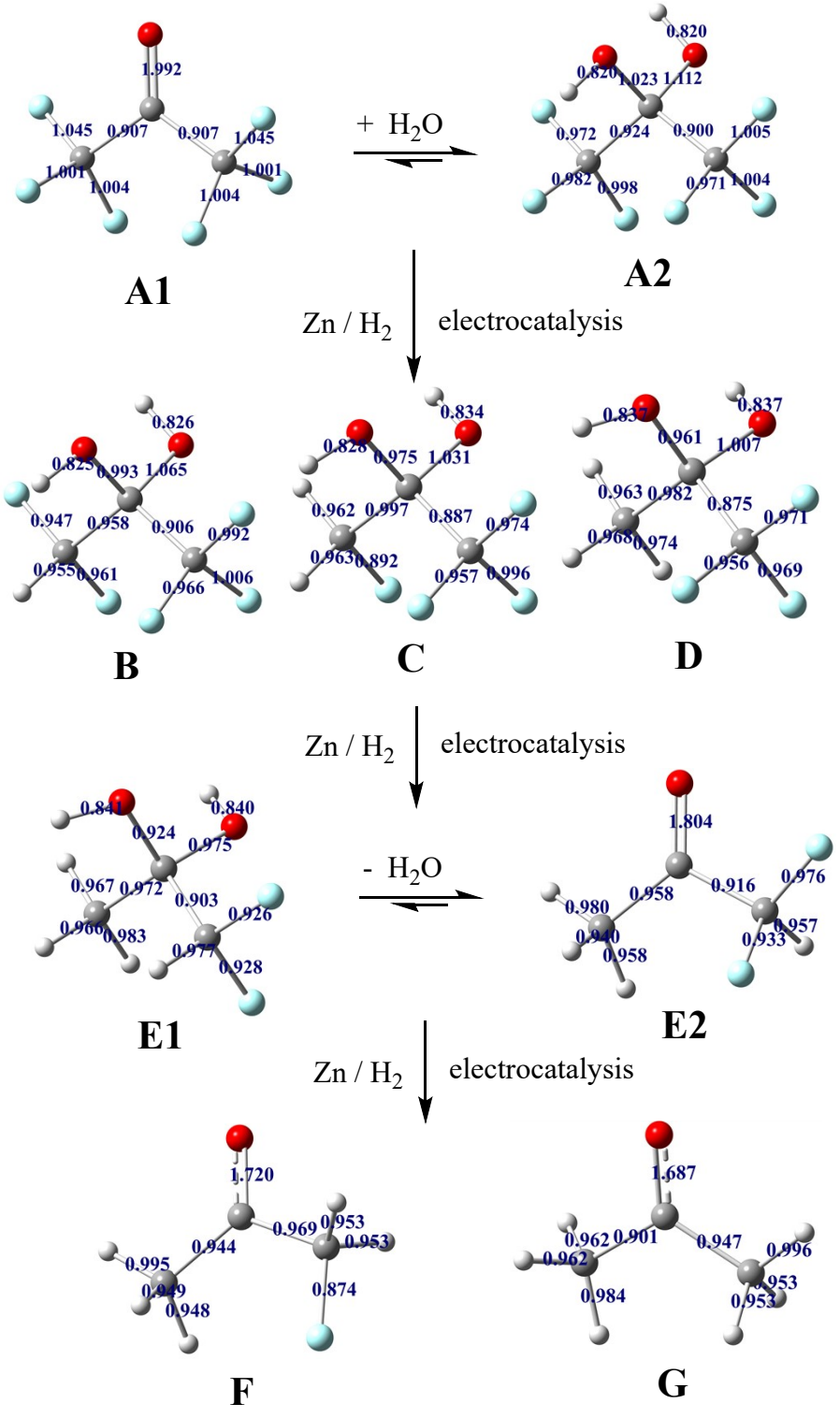
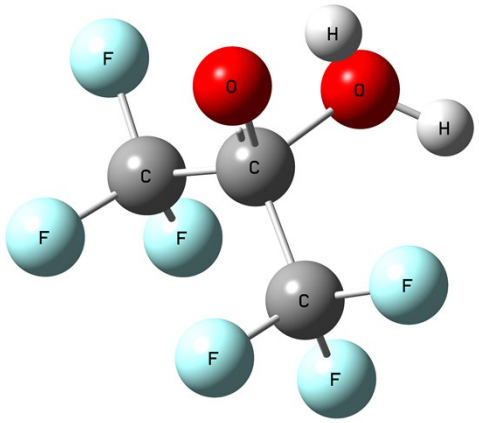
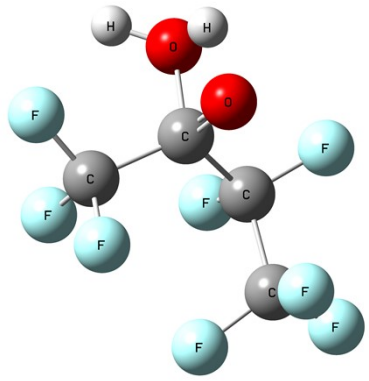


Fig S26 Structural diagrams and Cartesian coordinates of the TS (PF-A)



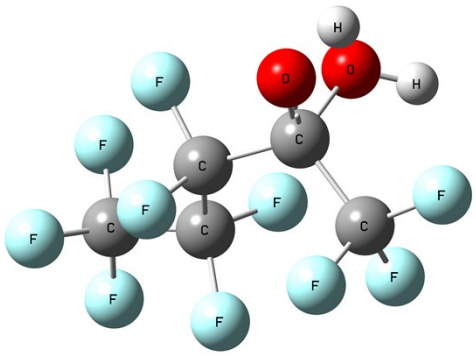
Center Number	Atomic	Coordinates (Angstroms) X	Y	Z
1	C	0.001931	0.566929	-0.166819
2	O	-0.010498	1.351069	-1.242909
3	F	2.375460	0.517386	-0.151009
4	F	1.395279	-0.841003	1.226621
5	F	-2.368769	0.538292	0.015031
6	C	1.304599	-0.269633	0.013471
7	C	-1.301331	-0.275169	0.009411
8	F	1.360718	-1.245523	-0.909989
9	F	-1.329462	-0.998199	1.141461
10	F	-1.429102	-1.119199	-1.025839
11	O	0.085142	1.676179	0.853541
12	H	-0.645258	1.763380	1.497781
13	H	-0.020207	2.220089	-0.185709

Fig S27 Structural diagrams and Cartesian coordinates of the TS (PF-2B)



Center Number	Atomic	Coordinates (Angstroms) X	Y	Z
1	O	1.401627	1.864041	0.289820
2	H	1.486597	1.985231	-0.882670
3	H	2.232488	1.728832	0.786990
4	C	-1.670169	-0.481164	-0.141210
5	C	0.747299	0.630380	-0.295820
6	O	0.860609	0.989020	-1.570620
7	F	2.872661	-0.430397	-0.157690
8	F	1.429852	-1.022159	1.352740
9	F	-1.308577	-1.631653	0.441710
10	F	-1.664779	-0.649254	-1.467090
11	F	-2.917410	-0.189495	0.247270
12	F	-1.276093	1.826197	-0.142260
13	C	1.568751	-0.644899	0.071280
14	C	-0.712291	0.671248	0.282130
15	F	1.174883	-1.662959	-0.709280
16	F	-0.690371	0.693948	1.639470

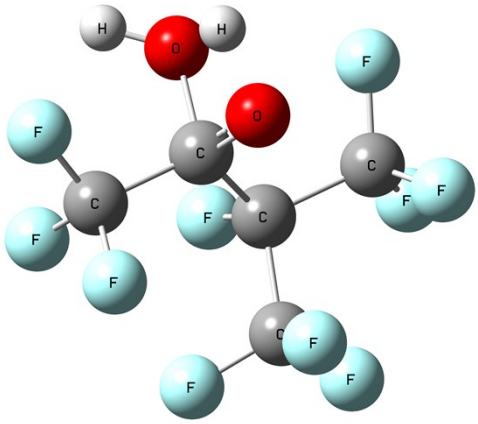
Fig S28 Structural diagrams and Cartesian coordinates of the TS (PF-2P)



Center Number	Atomic	Coordinates (Angstroms) X	Y	Z
1	C	-1.005599	-0.415000	-0.211930
2	C	2.228091	-0.650459	0.072910
3	F	3.508491	-0.482829	-0.279000
4	F	1.722881	-1.645239	-0.678580
5	F	2.195411	-1.045439	1.355770
6	F	-0.748199	-1.600820	0.384180
7	F	-0.781519	-0.540570	-1.538870
8	F	-0.574670	1.881220	0.093960
9	C	1.457710	0.700451	-0.071260
10	O	2.109600	1.735831	0.452630
11	H	2.094240	1.987911	-0.889980
12	O	1.464780	1.197831	-1.496120
13	H	1.930520	0.661751	-2.168270
14	C	-0.050910	0.664800	0.385470
15	F	-0.065220	0.523040	1.734880

16	C	-2.529299	-0.114671	-0.022010
17	F	-2.926800	0.866019	-0.836220
18	F	-2.792270	0.236159	1.241720
19	F	-3.229189	-1.217061	-0.312610

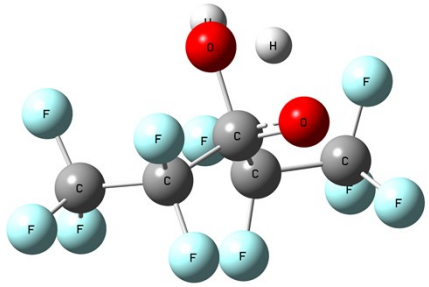
Fig S29 Structural diagrams and Cartesian coordinates of the TS (PF-3M2B)



Center Number	Atomic	Coordinates (Angstroms) X	Y	Z
1	O	0.854469	-2.075311	-0.497680
2	H	0.834239	-2.329781	0.660900
3	H	1.680449	-2.263341	-0.985300
4	C	-0.640428	1.475510	0.105500
5	C	0.770170	-0.740491	0.214480
6	O	0.650900	-1.233180	1.444120
7	F	3.146740	-0.820452	0.216740
8	F	2.265881	0.497728	-1.265690
9	F	0.246372	2.233240	-0.550920
10	F	-0.424778	1.600440	1.419420
11	F	-1.859708	1.961501	-0.166400
12	C	2.124491	0.018089	-0.019590
13	C	-0.511019	-0.018030	-0.353470
14	F	2.232161	1.038638	0.842030

15	F	-0.457209	0.002080	-1.727550
16	C	-1.825480	-0.788169	0.036930
17	F	-1.704651	-2.112969	-0.072240
18	F	-2.190020	-0.501078	1.294470
19	F	-2.817460	-0.412508	-0.784330

Fig S30 Structural diagrams and Cartesian coordinates of the TS (PF-3P)

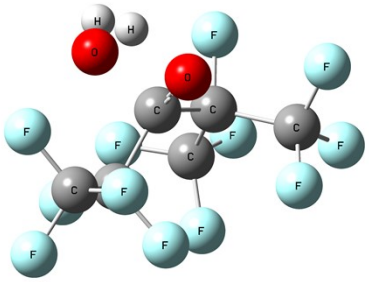


Center Number	Atomic	Coordinates (Angstroms) X	Y	Z
1	F	-0.867781	-1.260350	1.128820
2	F	-0.716361	-1.203940	-1.059330
3	F	1.711979	-1.770570	0.031950
4	F	2.519160	-0.342501	1.458860
5	F	2.069960	1.712220	-0.252660
6	C	-0.068220	0.788910	0.116450
7	O	-0.597810	1.922300	-0.336330
8	H	-0.426590	2.144300	0.997910
9	O	0.120200	1.250350	1.543970
10	H	-0.355540	0.762710	2.244450
11	C	1.389170	0.555060	-0.440280
12	F	1.306490	0.341420	-1.776820
13	C	2.283920	-0.567590	0.161820
14	C	-1.017140	-0.464170	0.035070
15	C	-2.538950	-0.124689	-0.079770
16	F	-2.817970	0.462371	-1.244650

17	F	-2.955870	0.659191	0.919920
18	F	-3.229771	-1.275779	-0.019620
19	F	3.459090	-0.590211	-0.482390

Fig S31 Structural diagrams and Cartesian coordinates of the TS (PF-2M3P Unbonded)

From a structural perspective, the transition state does not form the second C - O bond. Possibly, it is unable to form a stable existence.



Center Number	Atomic	Coordinates (Angstroms) X	Y	Z
1	C	1.676339	1.326659	-0.121581
2	C	1.220029	-0.056891	0.447219
3	C	1.814479	-1.250221	-0.391331
4	C	-1.342961	0.353859	-0.306461
5	F	-1.362451	1.703019	-0.176311
6	F	-0.961641	0.069919	-1.576801
7	F	1.017439	-1.584821	-1.409831
8	F	1.985749	-2.316411	0.391239
9	F	3.015509	-0.931691	-0.903911
10	F	1.816439	-0.141081	1.688449
11	F	1.094639	2.340519	0.530459
12	F	1.376579	1.428129	-1.423701
13	F	2.998969	1.474899	0.023369
14	C	-0.344761	-0.301631	0.711069

15	O	-0.730261	0.266489	2.065239
16	H	-0.005151	0.646559	2.599379
17	O	-0.617271	-1.568601	1.008229
18	H	-0.857531	-0.905261	2.164989
19	C	-2.822371	-0.140161	-0.184131
20	F	-3.582341	0.615799	-0.994351
21	F	-3.293971	-0.015521	1.059819
22	F	-2.945091	-1.410991	-0.572971

Table S1 Cartesian coordinates of the PF-A and gem diol

PF-A

Center Number	Atomic	Coordinates (Angstroms) X	Y	Z
1	C	0.000011	0.721805	-0.000007
2	O	0.000007	1.911163	0.000007
3	F	-2.335057	0.661597	-0.424236
4	F	-1.227265	-1.169963	-0.803823
5	F	2.335091	0.661564	0.424224
6	C	-1.326618	-0.096748	-0.004343
7	C	1.326615	-0.096734	0.004344
8	F	-1.591832	-0.517135	1.244474
9	F	1.591780	-0.517143	-1.244472
10	F	1.227272	-1.169948	0.803830

PF-A gem diol

Center Number	Atomic	Coordinates (Angstroms) X	Y	Z
1	C	-1.288138	-0.256838	-0.023832
2	F	-1.273444	-1.199436	-0.966563
3	F	-2.348706	0.543617	-0.246599
4	F	-1.476979	-0.855716	1.171583

5	F	2.379003	0.573176	0.054754
6	C	0.007107	0.626062	-0.013183
7	O	0.055731	1.406001	-1.144938
8	H	-0.617976	2.094717	-1.071550
9	O	-0.021857	1.444450	1.118685
10	H	-0.152345	0.913254	1.915523
11	C	1.313395	-0.226741	-0.019297
12	F	1.428823	-0.988083	-1.110439
13	F	1.325207	-1.036500	1.064366

Table S2 Cartesian coordinates of the PF-2B and gem diol

PF-2B

Center Number	Atomic	Coordinates (Angstroms) X	Y	Z
1	C	-1.523000	-0.533136	-0.197825
2	C	0.727706	0.839974	-0.258271
3	O	1.030964	1.788584	-0.908667
4	F	3.006266	0.212683	-0.081898
5	F	1.635904	-0.792280	1.268293
6	F	-0.986408	-1.663552	0.272627
7	F	-1.485790	-0.561721	-1.538427
8	F	-2.792482	-0.460944	0.200463
9	F	-1.410516	1.802386	-0.049087
10	C	1.776124	-0.277779	0.040449
11	C	-0.727649	0.702963	0.309587
12	F	1.614747	-1.267262	-0.857985
13	F	-0.666920	0.652823	1.664424

PF-2B gem diol

Center Number	Atomic	Coordinates (Angstroms) X	Y	Z
1	C	1.715524	-0.489528	0.128353

2	C	-1.679137	-0.529656	-0.116560
3	F	-2.878920	-0.343206	0.475822
4	F	-1.194161	-1.697724	0.324056
5	F	-1.869596	-0.614509	-1.432471
6	F	1.355199	-1.681091	-0.359043
7	F	1.831225	-0.574755	1.452384
8	F	2.915408	-0.176486	-0.383012
9	F	1.263036	1.811009	0.026038
10	C	-0.752310	0.655664	0.296163
11	O	-1.395977	1.785315	-0.196316
12	H	-0.852462	2.560272	-0.000312
13	O	-0.593573	0.668974	1.676970
14	H	-1.463178	0.786423	2.082371
15	C	0.697929	0.611758	-0.305722
16	F	0.615588	0.557824	-1.652740

Table S3 Cartesian coordinates of the PF-2P and gem diol

PF-2P

Center Number	Atomic	Coordinates (Angstroms) X	Y	Z
1	C	-0.873917	-0.338350	-0.257702
2	C	1.482453	0.808968	-0.254458
3	C	2.421293	-0.402953	0.045393
4	O	1.876926	1.730795	-0.893491
5	F	3.691549	-0.027029	-0.076539
6	F	2.171596	-1.375434	-0.850103
7	F	2.234067	-0.899001	1.274622
8	F	-0.465960	-1.505055	0.283618
9	F	-0.679251	-0.387946	-1.597786
10	F	-0.542165	1.987743	-0.023604
11	C	-2.406016	-0.197424	0.002024
12	C	0.014122	0.808346	0.306638
13	F	-2.916389	0.818874	-0.694400
14	F	-2.639266	0.001544	1.303499
15	F	0.066276	0.720639	1.658340
16	F	-3.014125	-1.325210	-0.378031

PF-2P gem diol

Center	Atomic	Coordinates (Angstroms)

Number		X	Y	Z
1	C	-1.036442	-0.460990	-0.182298
2	C	2.276324	-0.589765	0.125404
3	F	3.506159	-0.460154	-0.417561
4	F	1.734161	-1.709294	-0.372167
5	F	2.411129	-0.729333	1.443660
6	F	-0.791375	-1.563145	0.560147
7	F	-0.874963	-0.767149	-1.482801
8	F	-0.562487	1.864688	-0.122172
9	C	1.437525	0.661975	-0.274256
10	O	2.109990	1.734111	0.301746
11	H	1.632696	2.547092	0.088069
12	O	1.346327	0.752819	-1.657112
13	H	2.239994	0.833056	-2.016552
14	C	-0.040513	0.660932	0.264632
15	F	-0.005858	0.652621	1.614291
16	C	-2.544313	-0.092134	0.019374
17	F	-2.935010	0.828165	-0.865776
18	F	-2.763715	0.370325	1.255131
19	F	-3.282342	-1.192913	-0.162278

Table S4Cartesian coordinates of the PF-3M2B and gem diol

PF-3M2B

Center Number	Atomic	Coordinates (Angstroms) X	Y	Z
1	C	-1.140296	-1.255952	-0.230829
2	C	-0.605217	0.001553	0.536071
3	C	-0.959698	1.342031	-0.167879
4	C	0.925539	-0.118571	0.885121
5	C	2.022505	-0.056468	-0.224030
6	O	1.250923	-0.235084	2.022165
7	F	3.123334	-0.668820	0.201327
8	F	2.315808	1.230370	-0.477302
9	F	1.621305	-0.636283	-1.363506
10	F	-0.343106	1.459288	-1.348866
11	F	-0.570816	2.357403	0.615393
12	F	-2.278179	1.435201	-0.361989
13	F	-1.253181	0.020774	1.736584
14	F	-0.457591	-2.341921	0.178236
15	F	-1.001687	-1.143654	-1.553487
16	F	-2.429708	-1.445122	0.043827

PF-3M2B gem diol

Center	Atomic	Coordinates (Angstroms)

Number		X	Y	Z
1	C	0.614535	1.467171	0.096560
2	C	0.513672	-0.022037	-0.380087
3	C	1.830616	-0.779874	0.042444
4	C	-0.770082	-0.805498	0.118675
5	C	-2.119851	-0.020410	-0.008834
6	O	-0.667577	-1.114607	1.475353
7	H	-0.112332	-1.899647	1.567230
8	O	-0.845887	-1.923733	-0.701802
9	H	-1.703556	-2.349678	-0.571395
10	F	1.666566	-2.115460	0.057501
11	F	2.218431	-0.418201	1.276216
12	F	2.812307	-0.503258	-0.812590
13	F	0.414056	1.590415	1.410009
14	F	-0.285412	2.216983	-0.548618
15	F	1.829730	1.958603	-0.194684
16	F	0.505143	0.022732	-1.747717
17	F	-2.282617	0.483350	-1.235875
18	F	-2.253518	0.954568	0.887113
19	F	-3.123548	-0.909739	0.197890

Table S5Cartesian coordinates of the PF-3P and gem diol

PF-3P

Center Number	Atomic	Coordinates (Angstroms) X	Y	Z
1	C	0.000081	0.000163	0.799082
2	O	0.000036	0.000286	1.989465
3	F	1.588449	1.741541	0.718754
4	F	0.788584	1.075056	-1.209641
5	F	-1.999124	1.425467	-0.750365
6	F	-2.893257	0.606733	1.054313
7	F	-1.588229	-1.741295	0.719110
8	C	-1.179383	-0.665248	0.017188
9	F	-0.788487	-1.075177	-1.209451
10	C	-2.393687	0.295465	-0.144767
11	C	1.179499	0.665360	0.017128
12	C	2.393615	-0.295566	-0.144754
13	F	-3.344418	-0.281162	-0.878936
14	F	1.998575	-1.425831	-0.749463
15	F	2.893677	-0.606191	1.054344
16	F	3.344115	0.280490	-0.879663

PF-3P gem diol

Center	Atomic	Coordinates (Angstroms)

Number		X	Y	Z
1	F	-2.158006	1.451830	-0.637666
2	F	-0.826574	0.091752	-1.711721
3	F	1.150546	-1.664903	-0.869331
4	F	1.691807	-1.402231	1.221850
5	F	2.288958	1.275921	0.687582
6	C	-0.018346	1.044577	0.371074
7	O	-0.077482	2.421580	0.204280
8	H	0.696988	2.812457	0.631988
9	O	-0.104011	0.658369	1.706806
10	H	-0.864437	1.095607	2.111781
11	C	1.414383	0.578036	-0.100318
12	F	1.620317	0.977749	-1.371849
13	C	1.848295	-0.916146	-0.008916
14	C	-1.231933	0.479308	-0.482034
15	C	-1.999045	-0.720876	0.162263
16	F	3.144930	-1.001129	-0.337674
17	F	-2.642501	-0.313137	1.272768
18	F	-1.186090	-1.727243	0.483673
19	F	-2.912356	-1.170505	-0.702617

Table S6Cartesian coordinates of the PF-2M3P and gem diol

PF-2M3P

Center Number	Atomic	Coordinates (Angstroms) X	Y	Z
1	C	-1.874611	-1.097202	-0.249995
2	C	-1.174712	0.071990	0.524455
3	C	-1.286212	1.443335	-0.203943
4	C	0.306275	-0.268547	0.948237
5	C	1.390887	-0.715156	-0.080118
6	O	0.600237	-0.208027	2.099185
7	F	1.850838	-1.926026	0.302080
8	F	0.882515	-0.824322	-1.326339
9	F	-0.583072	1.465705	-1.340114
10	F	-0.813375	2.400398	0.604324
11	F	-2.564616	1.716239	-0.484850
12	F	-1.855849	0.217821	1.698033
13	F	-1.322737	-2.266019	0.133754
14	F	-1.748857	-0.984727	-1.573482
15	F	-3.171925	-1.132484	0.047014
16	C	2.594292	0.273509	-0.132560
17	F	2.135204	1.519783	-0.334459
18	F	3.280237	0.247659	1.008383
19	F	3.407478	-0.054399	-1.137669

PF-2M3P gem diol

Center	Atomic	Coordinates (Angstroms)

Number		X	Y	Z
1	C	-1.698899	-1.293715	-0.192736
2	C	-1.222981	0.044375	0.445743
3	C	-1.775077	1.295860	-0.327589
4	C	1.349057	-0.315214	-0.338459
5	F	1.376141	-1.677242	-0.367501
6	F	0.972056	0.109606	-1.560411
7	F	-1.037841	1.616789	-1.388207
8	F	-1.819372	2.348300	0.498925
9	F	-3.029937	1.067788	-0.750836
10	F	-1.849639	0.095084	1.674759
11	F	-1.124886	-2.337729	0.453352
12	F	-1.363831	-1.364371	-1.483370
13	F	-3.016566	-1.450104	-0.079062
14	C	0.352974	0.122598	0.798846
15	O	0.589880	-0.654939	1.926733
16	H	0.386736	-1.583853	1.755331
17	O	0.669949	1.429312	1.106780
18	H	0.310786	1.634466	1.980542
19	C	2.824367	0.167061	-0.132143
20	F	3.606568	-0.509159	-0.988829
21	F	3.256285	-0.074241	1.108058
22	F	2.947381	1.467345	-0.397538

Table S7Cartesian coordinates of defluorination product (B-F) in PF-3M2B gem diol

The compounds corresponding to the abbreviated letters in this section are the substances shown in Figure 4 of the main text.

B1

Center Number	Atomic	Coordinates (Angstroms) X	Y	Z
1	C	-2.008489	-0.039949	-0.153063
2	C	0.550159	-0.409341	0.261812
3	C	1.936425	0.132015	-0.209750
4	O	0.478719	-1.695674	-0.292472
5	H	-0.087612	-2.248405	0.267162
6	O	0.476955	-0.392524	1.650420
7	H	1.178750	-0.950791	2.019492
8	F	-2.323031	-0.417850	1.098641
9	F	-2.213867	-1.091169	-0.965707
10	F	-2.883925	0.922024	-0.509182
11	F	-0.558885	1.721608	0.381009
12	F	2.139087	1.400416	0.181220
13	F	2.055721	0.090378	-1.549281
14	F	2.926751	-0.616088	0.312603
15	C	-0.577910	0.505498	-0.289371
16	H	-0.414297	0.691573	-1.351752

B2

Center Number	Atomic	Coordinates (Angstroms) X	Y	Z

1	C	-1.887238	0.064730	0.083189
2	F	-2.309657	1.306806	-0.189727
3	F	-1.682120	-0.026708	1.410624
4	F	-2.871925	-0.792955	-0.232474
5	C	-0.619734	-0.277251	-0.715841
6	H	-0.841673	-0.157151	-1.779888
7	C	0.559472	0.636526	-0.369925
8	O	0.501162	1.826506	-0.473033
9	C	1.886377	-0.044261	0.093833
10	F	1.704282	-0.731134	1.234433
11	F	2.824278	0.880454	0.307369
12	F	-0.314286	-1.601422	-0.460809
13	F	2.338217	-0.894303	-0.845346

B1-B2 TS

Center Number	Atomic	Coordinates (Angstroms) X	Y	Z
1	C	-1.70425203	-0.35803771	-0.00568336
2	C	0.68607797	0.69292229	0.14014664
3	C	1.56204797	-0.58255771	-0.08091336
4	O	0.72647797	1.16144229	1.38830664
5	H	1.38369797	2.10106229	0.66106664
6	O	1.39260797	1.89441229	-0.49852336
7	H	2.27301797	1.72063229	-0.88378336
8	F	-1.92080203	-0.20658771	1.31135664
9	F	-1.29175203	-1.62132771	-0.21827336

10	F	-2.88907203	-0.20600771	-0.62723336
11	F	-1.27078203	1.90193229	-0.39088336
12	F	1.42985797	-1.09960771	-1.31639336
13	F	1.22947797	-1.53001771	0.80714664
14	F	2.86265797	-0.29441771	0.10605664
15	C	-0.69675203	0.65287229	-0.56413336
16	H	-0.58589203	0.46401229	-1.63205336

C1

Center Number	Atomic	Coordinates (Angstroms) X	Y	Z
1	C	-1.972724	-0.127921	-0.000971
2	F	-2.279481	0.692701	-1.030058
3	F	-2.198046	0.565492	1.137754
4	F	-2.870441	-1.139948	-0.026341
5	C	-0.565966	-0.667342	-0.082896
6	H	-0.462392	-1.234727	-1.012894
7	C	0.493624	0.400894	-0.036824
8	O	0.307991	1.587682	-0.019097
9	C	1.961368	-0.128180	-0.001371
10	F	2.204200	-0.759885	1.164988
11	F	2.836300	0.873464	-0.119540
12	F	2.186917	-1.005173	-0.998185
13	H	-0.414385	-1.371295	0.740477

C2

Center Number	Atomic	Coordinates (Angstroms) X	Y	Z
1	C	-1.619696	0.103728	0.160033
2	F	-1.940695	1.401723	0.266870
3	F	-1.270345	-0.341634	1.382667
4	F	-2.719188	-0.570976	-0.215377
5	C	-0.493347	-0.097307	-0.862439
6	H	-0.811652	0.329034	-1.816397
7	C	0.810507	0.584908	-0.437197
8	O	0.888066	1.779363	-0.344069
9	C	2.021007	-0.333397	-0.171974
10	H	2.290269	-0.949653	-1.029489
11	F	1.717067	-1.144513	0.894051
12	F	3.085275	0.432181	0.184935
13	F	-0.304777	-1.461433	-1.016713

D

Center Number	Atomic	Coordinates (Angstroms) X	Y	Z
1	C	-1.669522	-0.177882	0.057499
2	F	-2.104499	0.421468	-1.074082
3	F	-1.893090	0.688158	1.072680
4	F	-2.480856	-1.242476	0.268756
5	F	2.456743	-1.101875	-0.719183

6	F	2.583843	0.040571	1.162106
7	C	-0.230570	-0.617403	-0.028058
8	H	0.026268	-1.154847	0.889734
9	H	-0.136094	-1.331057	-0.852147
10	C	0.748416	0.507867	-0.241382
11	O	0.455853	1.663140	-0.438717
12	C	2.239740	0.130835	-0.165917
13	H	2.875354	0.867669	-0.653191

E

Center Number	Atomic	Coordinates (Angstroms) X	Y	Z
1	C	1.374304	-0.186664	-0.000022
2	F	1.715633	0.543749	1.087339
3	F	1.715712	0.544104	-1.087111
4	F	2.182842	-1.276249	-0.000169
5	C	-0.074171	-0.598088	-0.000136
6	H	-0.258306	-1.223442	-0.878543
7	H	-0.258329	-1.223857	0.877965
8	C	-1.051638	0.552847	0.000081
9	O	-0.728917	1.723937	0.000152
10	C	-2.522245	0.199054	0.000147
11	H	-2.989122	0.616512	0.894685
12	F	-2.728748	-1.187235	-0.000252
13	H	-2.989361	0.617071	-0.894001

F

Center Number	Atomic	Coordinates (Angstroms) X	Y	Z
1	C	-1.075181	-0.100411	-0.000360
2	F	-1.292929	0.760169	-1.023047
3	F	-1.221256	0.608097	1.145022
4	F	-2.099113	-0.993806	-0.028666
5	C	0.251012	-0.804303	-0.090546
6	H	0.304345	-1.538005	0.718098
7	H	0.278552	-1.362955	-1.030337
8	C	1.471546	0.098564	-0.026862
9	O	1.379157	1.314357	-0.009353
10	C	2.785620	-0.618742	0.020238
11	H	2.864678	-1.142440	0.978891
12	H	2.831606	-1.378565	-0.764528
13	H	3.609264	0.086324	-0.081892