

Supporting information file for:

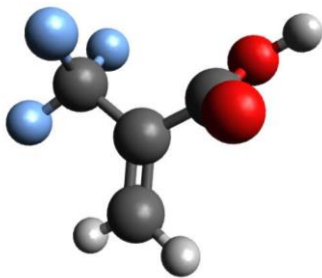
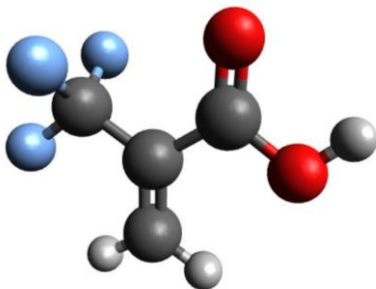
Study of low-energy electron interaction with 2-(trifluoromethyl) acrylic acid (TFMAA), a potential component for EUVL resist material

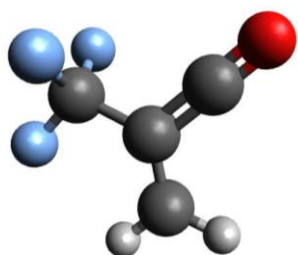
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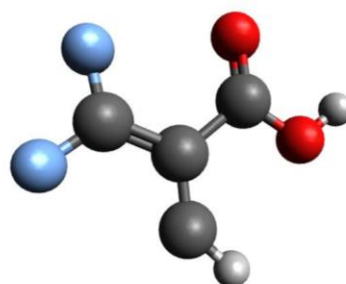
² Université Paris-Saclay, CNRS, Institut des Sciences Moléculaires d'Orsay, 91405 Orsay, France

Table S1: Positively charged and neutral structure of all the fragments along with their XYZ-outputs.

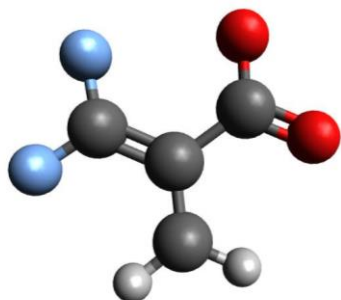
140: [C ₂ H ₂ CF ₃ COOH] ⁺	140: Neutral
	
O -0.617288 1.490195 -0.407922	O 0.159257 0.352894 -0.784879
C 0.049277 0.643123 0.295074	C -0.039282 0.930368 0.422342
H -0.064112 1.992245 -1.041153	H 0.492846 1.047819 -1.373483
O 1.241496 0.372871 0.262370	O 0.186642 2.091793 0.635808
C -0.606841 -0.153513 1.366870	C -0.562885 -0.032133 1.434527
C -1.103825 0.625113 2.602853	C -0.829375 0.538411 2.811779
C -0.630196 -1.509240 1.269820	C -0.794014 -1.312547 1.162146
H -0.120813 -2.027930 0.466055	H -0.604748 -1.706464 0.174206
H -1.183896 -2.098396 1.992875	H -1.174543 -1.986909 1.916127
F -2.039648 1.491450 2.220975	F -1.749325 1.517375 2.772672
F -1.613359 -0.215367 3.492545	F -1.297399 -0.407896 3.653036
F -0.080586 1.287570 3.137788	F 0.284914 1.041651 3.368190

123: [C₂H₂CF₃CO]⁺

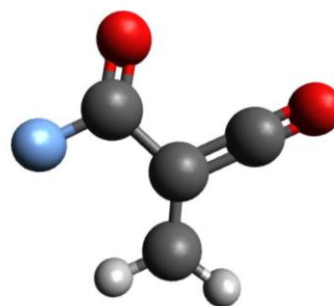
C	0.045092	0.975997	0.708518
O	0.503452	1.745209	0.037691
C	-0.532536	0.030483	1.561745
C	-0.886484	0.532637	2.984656
C	-0.736096	-1.217503	1.101258
H	-0.469225	-1.519005	0.094908
H	-1.184431	-1.958822	1.754488
F	-1.749922	1.541043	2.892061
F	-1.421823	-0.462141	3.670780
F	0.220563	0.960041	3.586975

120: [C₂HCF₂COOH]⁺

O	-0.047652	0.402033	-0.866171
C	-0.216018	1.085662	0.256827
H	0.066153	1.014034	-1.616714
O	-0.236578	2.265356	0.408662
C	-0.388801	0.094420	1.425912
C	-0.570542	0.600948	2.738958
C	-0.377199	-1.231843	1.269836
H	-0.271138	-1.947774	0.464771
F	-0.614349	1.824948	3.014923
F	-0.704526	-0.155734	3.743757

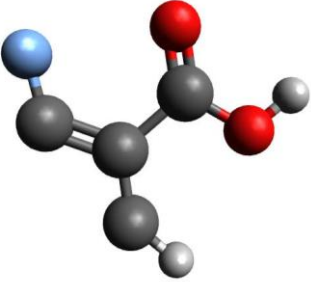
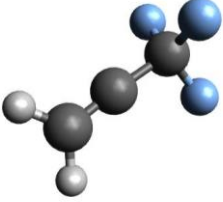
120: [C₂H₂CF₂COO]⁺

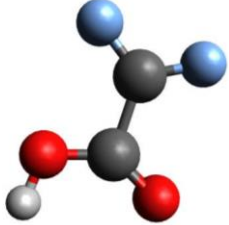
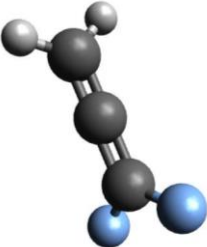
O	0.252258	0.466229	-0.716491
C	-0.138354	0.892054	0.384764
O	-0.045698	2.124321	0.539778
C	-0.681911	-0.052886	1.432000
C	-1.121166	0.443007	2.681379
C	-0.752232	-1.385973	1.179058
H	-0.413680	-1.763496	0.218287
H	-1.133659	-2.101142	1.899283
F	-1.078019	1.662314	2.988296

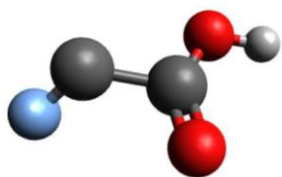
101: [C₂H₂CF₂COO]⁺

O	0.455238	0.970832	-0.887537
C	0.023715	0.462067	0.007983
O	-0.433413	1.910130	2.252014
C	-0.511187	-0.181096	1.142166
C	-0.673729	0.758411	2.312379
C	-0.814216	-1.493581	1.079551
H	-0.670511	-2.087690	0.183963
H	-1.221968	-1.984415	1.957210
F	-1.110279	0.112853	3.377351

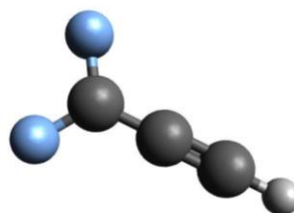
F	-1.593219	-0.299518	3.591405
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101: $[\text{C}_2\text{HCF}_2\text{COOH}]^+$	95: $[\text{C}_2\text{H}_2\text{CF}_3]^+$
	
O -0.047650 0.402030 -0.866170 C -0.216020 1.085660 0.256830 H 0.066150 1.014030 -1.616710 O -0.236580 2.265360 0.408660 C -0.388800 0.094420 1.425910 C -0.570540 0.600950 2.738960 C -0.377200 -1.231840 1.269840 H -0.271140 -1.947770 0.464770 F -0.614350 1.824950 3.014920	C -0.814996 -0.473205 1.925947 C -0.848982 0.642425 2.952491 C -0.815158 -1.445161 1.128059 H -0.435905 -1.328695 0.101248 H -1.189668 -2.437256 1.419258 F -1.688831 1.583307 2.595115 F -1.287475 -0.019798 4.026117 F 0.353646 1.129872 3.144454

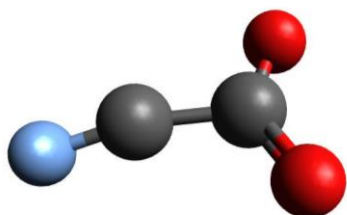
95: $[\text{C}_2\text{HF}_2\text{O}_2]^+$	76: $[\text{C}_2\text{H}_2\text{CF}_2]^+$
	
O -0.546178 0.712994 -0.177031 C 0.170167 1.276921 0.760058 H -0.167996 0.855642 -1.067705 O 1.167144 1.914753 0.777547 C -0.525178 0.989931 2.131308 F -1.579404 0.345593 2.256771 F -0.012875 1.424485 3.171473	C -0.990986 -0.536880 1.942528 C -1.168868 0.462518 2.863224 C -0.827259 -1.468245 1.081714 H -0.063878 -1.398325 0.300824 H -1.444547 -2.371733 1.091732 F -1.856277 1.504385 2.615730 F -0.660475 0.418119 4.028738

76: [CFCOOH]⁺

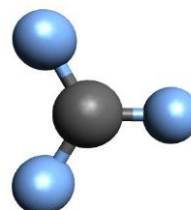
O	0.817697	0.542815	-0.079725
C	-0.067235	1.129680	0.643052
H	0.903603	0.922149	-0.980617
O	-0.852403	2.014927	0.532981
C	-0.270974	0.474054	2.040754
F	-0.041337	1.044325	3.094125

75: [C₃HF₂]⁺

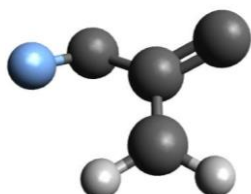
C	-1.032724	-0.535578	2.086128
C	-1.177104	0.523732	2.944357
C	-0.906570	-1.468694	1.328723
H	-0.794830	-2.297775	0.655018
F	-1.468184	1.682704	2.545961
F	-1.028129	0.411912	4.190103

75: [CFCOO]⁺

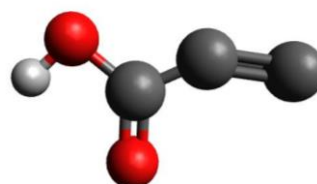
O	-0.12823	0.11680	-0.11777
C	-0.02260	1.11674	0.65238
O	0.12583	2.33217	0.32852
C	-0.08069	0.82426	2.13732
F	-0.39473	0.43278	3.35600

69: [CF₃]⁺

C	-0.897648	0.672459	3.151118
F	-1.715082	1.465693	2.670745
F	-1.270271	-0.442350	3.533251
F	0.291811	0.993727	3.250566

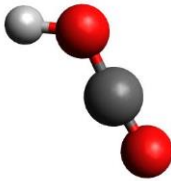
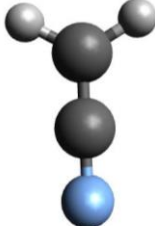
69: [C₂H₂CFC]⁺

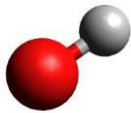
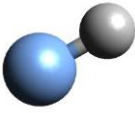
C	0.12399	0.60029	0.52930
C	-0.63267	0.03731	1.48345
C	-1.20351	0.58700	2.84325


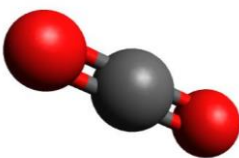
69: [CCCOOH]⁺

O	0.29521	0.41203	-1.19331
C	0.03226	0.83887	0.07927
H	0.61304	1.25299	-1.56923

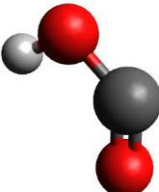
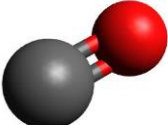
C	-0.80563	-1.28147	1.09041	O	0.19179	1.99648	0.52057
H	-0.70608	-1.60836	0.05891	C	-0.43063	-0.05827	0.90741
H	-1.07759	-2.03472	1.83151	C	-1.03901	-0.31550	2.22124
F	-1.00075	-0.27723	3.73735				

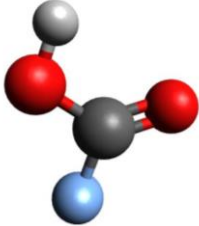
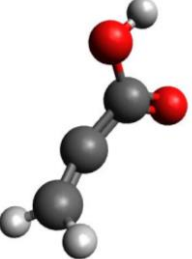
45: $[\text{COOH}]^+$		45: $[\text{C}_2\text{H}_2\text{F}]^+$					
O	0.163971	0.456562	-0.713743	C	-0.344823	-0.201153	1.973372
C	0.118842	1.289601	0.175121	C	-0.730539	-1.227962	1.351509
H	0.477129	0.700101	-1.620445	H	-0.525187	-1.333141	0.280338
O	0.039517	1.976606	1.058847	H	-1.275686	-2.018548	1.879214
				F	0.024954	0.784395	2.570756


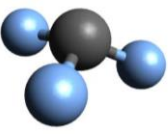
OH		HF					
O	0.051485	0.349029	-0.799532	F	-4.142426	1.660500	0.000000
H	0.232015	1.097391	-1.401098	H	-3.217694	1.660500	0.000000

F_2		CO_2					
F	-1.694213	3.310000	0.000000	O	0.084587	0.221063	-0.635473
F	-0.297557	3.278860	0.000000	C	0.102208	1.125020	0.091090

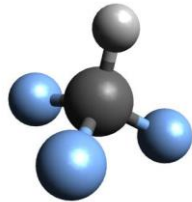
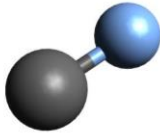
	O	0.119825	2.028977	0.817653
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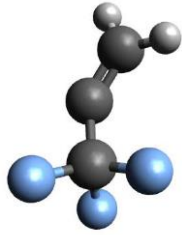
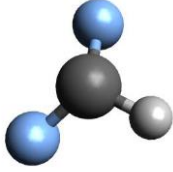
COOH		CO					
O	0.154440	0.357696	-0.765732	O	-3.056178	0.172640	0.000000
C	-0.018901	0.975054	0.392429	C	-1.931082	0.172640	0.000000
H	0.495149	0.990814	-1.431079				
O	0.168772	2.099305	0.704162				

FCOOH		C₂H₂COOH					
O	0.283750	0.344636	-0.170009	O	0.619132	0.647140	-0.996814
C	0.189697	1.255233	0.795710	C	-0.080200	0.793059	0.158394
H	0.317450	0.817668	-1.014764	H	0.747537	1.539332	-1.356396
O	0.152072	2.435658	0.698247	O	-0.436774	1.873239	0.586476
F	0.141401	0.611346	1.958795	C	-0.309808	-0.442296	0.821768
				C	-0.911580	-1.491509	1.276807
				H	-1.926585	-1.749424	0.971434
				H	-0.435181	-2.168561	1.982370

H₂		CF₃					
H	-1.097526	-0.308611	0.000000	C	-0.844333	0.561206	2.880149

H	-0.353794	-0.328839	0.000000	F	-1.747713	1.516620	2.746984
				F	-1.295625	-0.426542	3.633055
				F	0.296481	1.038246	3.345492

HCF₃		CF					
C	-0.828602	0.566388	2.821566	C	-0.583764	0.476513	2.548773
F	-1.750045	1.539670	2.783071	F	-1.386796	-0.248003	1.871987
F	-1.286609	-0.422074	3.601900				
F	0.288484	1.060551	3.373542				
H	-0.625007	0.195744	1.816381				

C₂H₂CF₃		CHF₂					
C	-0.654341	-0.151028	1.579114	C	-0.229508	0.216123	2.485844
C	-0.850686	0.562605	2.855542	F	-1.470851	0.075095	2.029949
C	-0.783802	-1.364092	1.127771	F	-0.098248	1.337262	3.188771
H	-0.561646	-1.621617	0.097326	H	0.167167	-0.669330	2.981156
H	-1.123345	-2.174354	1.774387				
F	-1.728158	1.574831	2.725400				
F	-1.328079	-0.260092	3.820782				
F	0.302687	1.085238	3.312367				

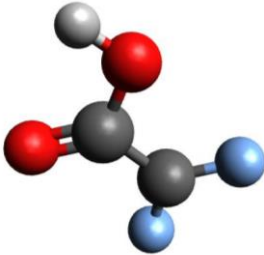




CF ₂ COOH				CF ₂			
							
O	0.554141	0.064756	0.281852	C	-0.756078	0.723533	2.569452
C	0.317691	1.092735	1.132417	F	-0.906867	-0.452935	2.027906
H	1.085853	0.423364	-0.445154	F	0.433574	0.693453	3.102478
O	0.718060	2.227031	0.980554				
C	-0.465554	0.678154	2.262818				
F	-0.948625	-0.528330	2.428363				
F	-0.845875	1.525080	3.180539				

Table S2: Comparison of appearance energies (AEs) and threshold values calculated at the B3LYP and the DLPNO-CCSD(T) level of theory for potential reactions leading to the respective m/z ratios in DI of TFMAA.

Fragment	Product	AE (eV)	B3LYP (eV)	DLPNO-CCSD(T) (eV)
95	[C ₂ HF ₂ O ₂] ⁺ + C ₂ H + HF	13.2 ± 0.3	15.81	15.83
	[C ₂ HF ₂ O ₂] ⁺ + C ₂ H ₂ F		13.35	13.73
	[C ₂ HF ₂ O ₂] ⁺ + C ₂ H ₂ + F		17.32	17.52
76	[C ₂ HFO ₂] ⁺ + C ₂ H ₂ + F + F	11.2 ± 0.3	20.99	21.33
	[C ₂ HFO ₂] ⁺ + C ₂ H ₂ + F ₂		19.45	19.89
	[C ₂ HFO ₂] ⁺ + C ₂ H ₂ F ₂ (Difluoroethylene) 		13.45	14
	[C ₂ HFO ₂] ⁺ + C ₂ H ₂ F ₂ (Cis-Difluoroethylene) 		13.87	14.44
	[C ₂ HFO ₂] ⁺ + C ₂ H ₂ F ₂ (Trans-Difluoroethylene) 		13.90	14.47
75	[C ₂ FO ₂] ⁺ + C ₂ H ₂ + HF + F	13.2 ± 0.2	18.94	19.04
	[C ₂ FO ₂] ⁺ + C ₂ H ₂ + H + F + F		24.62	24.63
	[C ₂ FO ₂] ⁺ + C ₂ H + HF + HF		17.43	17.35