Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for

Detailed Kinetics of Tetrafluoroethene Ozonolysis

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Table S1: The optimized geometries, electronic energies at 0 K ($E_{elec}^{0\,K}$), zero-point energy (ZPE) corrections, harmonic wavenumbers and anharmonic coefficients of the species involved, calculated at CCSD(T)/CBS/B3LYP/aug-cc-pVTZ level of theory for the title reaction.

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1}) and anharm. coefficients (cm^{-1})
O_3 (C_{2v})	O	0.000000000	0.429028000	0.000002000	-225.247587	0.007252	Freqs. 1248.857 1188.788 745.641 Anharm. coefficients -3.741 -18.274 -3.444 -5.741 -11.048 -0.951 (705.0^1; 1042.0^2; 1110.0^1)
	O	1.077373000	-0.214514000	0.000010000			
	O	-1.077373000	-0.214514000	-0.000012000			
C_2F_4 (D_{2h})	C	0.000000000	0.000000000	0.660406000	-475.194223	0.021425	Freqs. 1905.589 793.443 397.732 199.173 1181.349 552.946 554.566 1319.397 210.403 1322.047 552.687 415.568 Anharm. coefficients -7.406 -2.382 -0.630 -1.729 -0.198 0.049 -0.758 -0.175 -0.171 0.039 -4.819 -3.387 -1.444 -0.415 -1.739 -0.118 -0.059 0.050 -0.098 -3.477
	F	0.000000000	1.100785000	1.387870000			
	F	0.000000000	-1.100785000	1.387870000			
	C	0.000000000	0.000000000	-0.660406000			
	F	0.000000000	-1.100785000	-1.387870000			
	F	0.000000000	1.100785000	-1.387870000			

Species	Cartesian coordinate (Å)			$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1}) and anharm. coefficients (cm^{-1})
						-18.671 -2.822 -0.264 -2.093 -0.735 -3.992 -4.118 -1.716 -0.709 -6.900 -0.914 -0.299 0.236 0.269 0.496 -9.848 -3.796 -1.863 -0.738 -5.968 -4.072 -1.156 0.083 -1.002 -1.124 -2.847 -14.884 -0.476 0.591 -1.053 0.128 0.605 1.772 -3.188 -4.178 -2.538 0.215 -1.472 -1.376 1.006 -3.872 -5.305 -11.967 -2.393 -1.822 -0.334 -0.199 -2.469 -0.030 -1.091 -0.048 -1.253 -2.081 0.468 -2.184 0.017 -0.950 0.530 (190; 218; 394; 406; 508; 551; 558; 778; 1186; 1337; 1340; 1872)[3]
Pre-complex (C_s)	C -1.108785000 -0.661414000 0.005061000 C -1.108675000 0.661528000 0.004827000 O 2.069766000 -1.076945000 -0.159421000 O 2.548492000 -0.000263000 0.277030000 O 2.070156000 1.076866000 -0.158738000 F -1.116536000 -1.388011000 -1.092910000 F -1.117176000 -1.385010000 1.108382000 F -1.116308000 1.387737000 -1.093398000 F -1.116930000 1.385512000 1.107893000			-700.445562	0.029159	Freqs. 1869.181 1328.079 1324.551 1230.668 1193.048 1171.013 793.775 745.539 554.232 553.019 551.339 414.005 396.823 211.321 201.138 112.193

Species	Cartesian coordinate (Å)	$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1}) and anharm. coefficients (cm^{-1})
				35.200 35.186 32.968 30.120 16.017 Anharm. coefficients -13.518 -6.457 -2.248 -0.906 -12.582 -2.846 -9.482 1.578 1.487 -5.402 -2.522 -3.002 -3.571 -8.547 -1.298 -4.328 -2.695 -3.061 -9.752 -5.824 -2.417 -3.992 -4.153 -0.001 -1.857 -0.502 0.128 0.058 -5.889 -5.414 0.182 -3.886 -3.298 0.210 -2.034 -4.381 -1.115 -2.545 -0.029 -0.663 -17.887 -4.624 -4.107 -0.064 -0.189 -2.264 -2.165 -2.046 -0.057 -0.699 -1.888 -2.071 -1.746 -0.190 -0.826 -1.010 -2.386 -1.616 0.080 0.146 -1.283 -0.711 -0.923 -0.168 -0.409 25.154 -4.612 -4.037 13.793 0.177 0.432 0.293 -0.281 0.333 -0.263 -1.694 0.948 0.361 -0.529 -0.074 -0.001 0.397 -0.223 0.296 -0.227 -1.332 1.813 0.679 0.052 0.236 -1.508 3.149 0.733 1.426 5.214 -1.469 -1.619 -0.635 -5.726 0.008 -0.920 -1.663 -0.126 0.035 0.128 -0.581 -1.193 0.014 -0.376 -0.017 -0.391 -2.753 0.414 1.221 0.022 -0.719 -17.427 -0.104 -0.138 -0.977

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1}) and anharm. coefficients (cm^{-1})
							-0.767 -2.821 -0.010 0.019 -0.145 0.319 -0.420 -0.030 0.220 -0.146 -0.392 -0.280 -0.043 -0.131 -1.131 3.881 -0.211 0.659 -0.137 1.546 -0.223 -0.252 -0.385 0.013 -0.261 0.483 -0.214 0.214 0.259 0.270 -0.210 -0.239 0.536 -0.500 -0.542 0.461 0.169 0.669 -0.003 0.101 5.643 -1.361 0.041 -0.286 0.078 2.478 -0.741 0.263 -2.488 1.816 -0.045 0.270 0.454 0.142 0.976 -0.036 0.755 0.074 -0.179 0.590 1.988 4.400 0.547 -0.922 2.820 3.161 0.785 0.570 0.741 0.746 3.252 1.770 0.004 -1.395 -1.530 3.087 0.343 0.649 -0.559 -2.397 13.254 -1.089 0.063 -0.324 -0.336 36.080 4.915 -0.089 -3.225 -1.059 -33.693 -6.275 1.272 -19.942 -1.229 -3.167 8.395 -16.046 -7.688 1.800 -12.603 -15.416 -30.205 -0.670 -3.270 -65.829 -2.977 -6.023 17.018 -40.011 23.374
TS1 (C_s)	C	0.693710000	0.683833000	0.016828000	-700.431592	0.030042	Freqs. -325.588 HO 1661.589 1362.251 1355.559 1188.985 1112.622
	C	0.693809000	-0.683769000	0.016841000			
	O	-1.510065000	1.067613000	-0.240409000			
	O	-1.982728000	-0.000093000	0.300408000			
	O	-1.510026000	-1.067749000	-0.240457000			
	F	0.937880000	1.372848000	-1.065949000			
	F	0.822930000	1.358336000	1.134899000			

Species	Cartesian coordinate (Å)			$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1}) and anharm. coefficients (cm^{-1})
	F 0.938066000	-1.372781000	-1.065917000			1077.636
	F 0.823061000	-1.358240000	1.134928000			790.392
						753.349
						577.267
						561.390
						550.359
						466.099
						400.661
						301.281
						242.232
						211.879
						193.271
						162.312
						157.722
						59.962
						Anharm. coefficients
						-16.187
						14.071 -3.460
						-3.118 -6.348 -3.120
						-2.185 -2.130 -13.890 -3.294
						-0.368 -8.351 -7.040 -7.273 -1.951
						7.253 0.404 -0.169 0.506 -0.411
						7.088 1.081 -0.330 -0.185 -0.487
						0.329 -2.427 -5.752 -4.115 -3.209
						-1.729 -1.525 -0.545 -0.131 -0.502
						-2.946 -7.842 -6.524 -4.011 -2.004
						-1.390 -10.239 -5.243 -4.026 1.173
						-0.231 -4.048 -1.958 -2.723 -1.109
						-18.370 -5.334 -0.329 0.316 -0.082
						0.802 -1.103 -2.974 -2.109 -1.553
						3.437 -1.369 -2.930 -2.017 -1.176
						-3.920 -2.030 -1.738 -1.091 -0.853
						-0.615 -0.574 -4.903 -2.468 0.440
						-7.111 -2.463 -1.172 0.332 -0.287

Species	Cartesian coordinate (Å)	$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1}) and anharm. coefficients (cm^{-1})				
				-6.221	-2.753	-2.540	-1.014	-1.253
				-5.657	-2.270	-2.468	-0.832	-0.937
				5.986	1.670	-4.366	-0.585	-0.539
				-2.155				
				-13.389	-3.545			
				0.861	-0.249	-0.595		
				-5.459	-9.518	-0.066	-0.713	
				-2.227	-2.190	-0.225	-0.550	-0.052
				-2.432	-1.590	-1.924	-0.978	0.367
				-0.367	-0.576	-2.058	-0.214	-0.948
				-1.193	-5.949	0.083	-1.324	-0.118
				-0.579	-0.639	-4.608	-0.668	-1.066
				-0.024	-0.826	0.814	-0.647	-1.277
				-1.277	-1.800	-0.772	-0.304	-1.297
				-0.814	-1.215	-0.289	-0.544	-5.489
				-3.317	-4.089	0.554	-1.061	-2.443
				-1.333	-2.064	-0.398	-0.140	-5.394
				-1.431	-2.510	0.375	-0.817	-2.252
				-0.721	-1.824	1.941	0.635	-5.012
				0.285				
				-0.923	-0.088			
				0.430	0.204	2.180		
				-1.421	-0.455	0.833	0.970	
				-1.249	-0.246	0.422	0.081	0.074
				-1.439	0.479	3.455	-0.160	0.096
				-5.199	-0.556	2.082	-0.555	0.359
				-5.407	-0.959	7.555	1.425	-1.218
				-5.511	-0.514	3.980	0.455	-7.541
				-2.346	-0.820	4.810	1.115	-0.692
				-3.457	0.318	8.620	6.707	6.786
				0.333				
				0.656	0.779			
				1.095	0.863	0.239		
				-0.761	-1.949	1.502	1.315	

Species	Cartesian coordinate (Å)			$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1}) and anharm. coefficients (cm^{-1})
						0.377 1.026 0.976 1.439 1.168 5.260 9.510 6.649 11.140 7.581 9.092
TS2 (C_s)	C 1.021487000 0.285877000 0.030455000 C -0.690480000 -0.527688000 -0.023281000 O 0.767097000 1.468121000 0.254072000 O -1.313830000 1.559141000 0.017160000 O -1.338364000 0.452091000 -0.682048000 F 1.553121000 -0.090010000 -1.156709000 F 1.596450000 -0.489243000 0.980852000 F -0.686106000 -1.648322000 -0.696787000 F -1.008494000 -0.703975000 1.233030000			-700.537462	0.031044	Freqs. -496.491 HO 1531.521 1331.767 1293.981 1146.537 1109.771 951.022 854.004 733.492 682.391 585.957 558.267 515.046 502.607 461.469 330.471 282.523 268.864 206.763 192.954 87.322 Anharm. coefficients -5.693 1.509 -2.389 1.562 1.041 -6.640 5.778 4.435 -7.248 -5.558 -8.708 -0.230 -2.464 -2.006 -6.826 4.285 -3.207 0.591 -1.345 0.680 -0.364 -2.777 -3.323 -8.320 -0.257 2.217 -0.719 -0.840 -8.348 0.754

Species	Cartesian coordinate (Å)	$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1}) and anharm. coefficients (cm^{-1})				
				0.464	-2.447	-3.200	-3.054	-0.655
				-1.018	-2.333	-6.960	-3.697	-3.901
				-0.253	-4.787	-0.350	-0.528	-0.079
				0.505	0.212	-0.423	-0.664	-0.411
				6.375	-5.047	-3.199	-8.243	0.650
				0.894	-2.909	-2.965	-3.849	-1.224
				4.326	-6.714	-2.117	-5.025	-1.920
				-1.476	-3.214	-1.251	-1.504	-1.308
				0.415	-2.991	-1.577	-2.815	-0.198
				-1.936	-1.298	-1.987	-2.280	0.001
				0.539	-2.440	-1.245	-2.188	-0.162
				-0.121	-2.420	-2.099	-2.348	1.054
				0.862	-0.797	-1.588	-2.216	0.262
				-5.722				
				-5.582	-1.227			
				-6.057	-4.309	-0.949		
				-3.118	0.827	-1.562	-0.404	
				-0.327	-0.852	-0.346	-0.154	-0.132
				-2.697	-1.081	-1.537	0.014	-0.049
				-5.874	-2.800	-2.367	-0.326	-0.125
				-1.259	-0.279	1.454	-0.971	-0.935
				-1.757	-0.577	-1.002	-0.160	-0.364
				-1.474	1.246	-2.408	-0.568	0.309
				-1.190	-1.329	-1.523	-0.422	-0.261
				-1.156	-0.201	-2.203	-0.455	-0.304
				-0.351	-0.563	-1.884	-0.481	-0.298
				-1.591	0.811	-0.769	-1.075	-0.017
				-0.456	-1.745	-0.623	-0.061	0.485
				-0.054	-0.238	-0.788	-0.441	-0.232
				-0.092				
				0.022	-0.002			
				-0.691	-0.121	-0.426		
				-0.319	0.019	-0.489	-0.339	
				-0.137	0.500	1.053	0.119	0.255

Species	Cartesian coordinate (Å)			$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1}) and anharm. coefficients (cm^{-1})
						-0.573 0.664 -0.068 0.155 0.627 1.158 0.104 1.186 0.859 0.031 0.330 0.232 0.069 -0.110 0.554 0.073 0.283 0.025 0.922 0.609 0.026 0.363 0.783 1.054 -0.062 -0.085 0.417 -1.904 -0.389 -1.974 0.103 0.520 0.154 0.509 0.691 0.062 0.609 -0.670 -0.099 -0.090 0.069 0.203 -0.304 -0.842 0.267 -0.042 -0.397 -0.978 -0.939 -1.187 0.163
Adduct (C_s)	C 0.791830000 -0.226859000 -0.001794000 C -0.791960000 -0.226520000 -0.001759000 O 1.124687000 1.060438000 -0.408925000 O 0.000631000 1.826940000 0.073619000 O -1.124360000 1.061174000 -0.408048000 F 1.307752000 -1.085064000 -0.879492000 F 1.276121000 -0.519127000 1.211455000 F -1.308164000 -1.083980000 -0.880068000 F -1.276473000 -0.519401000 1.211233000			-700.583537	0.033959	Freqs. 1327.590 1240.673 1200.604 1164.777 1132.161 1074.051 963.003 811.963 764.938 705.749 663.303 645.293 565.817 544.461 494.186 394.587 329.119 317.053 265.485 237.563

Species	Cartesian coordinate (Å)	$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1}) and anharm. coefficients (cm^{-1})
				63.936 Anharm. coefficients -3.276 -7.726 -3.458 -3.247 -6.757 -3.155 -1.844 0.183 -11.278 -3.276 -2.656 -0.906 0.777 -2.005 -3.649 -3.127 -1.286 -0.423 -1.826 -11.554 -1.558 -1.536 -0.582 -1.050 -1.897 -4.916 -2.392 -0.882 -0.961 -5.966 -1.371 -2.999 -3.514 -2.957 -2.050 -2.095 -1.591 0.435 -0.791 -2.243 -2.184 -2.011 -5.627 0.073 -1.315 -1.942 -1.874 -1.920 -1.596 -2.943 -3.594 -1.882 -3.788 -1.716 -2.062 -0.647 -0.980 -2.395 -2.508 -1.468 -1.473 -2.850 -1.534 1.954 -1.744 -1.163 -1.219 -1.108 -0.792 -1.161 -1.630 -1.512 -1.116 -0.657 -2.010 -1.669 -0.881 -1.094 -0.589 0.335 -1.071 -1.333 -1.061 -0.768 0.223 -2.298 -0.853 -0.815 -0.141 -0.427 1.328 -1.158 0.709 0.960 -0.975 -2.463 -0.772 -2.705 -1.852 -10.401 -4.504 -1.917 -1.558 -2.311 -0.435 -2.196 -5.066 -4.689 -0.431 -0.279 -0.819 -3.306 -2.382 -0.571 -0.725 -1.551 -0.861 -0.703 -0.389 -0.979 -0.926 -0.946 -1.376 0.088 -0.832 -1.311 -0.454 0.753 -1.296 -0.295 -1.304 -0.473 -0.949 0.996 -0.898 -0.696 -1.103 -0.183 -1.711 -0.499

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1}) and anharm. coefficients (cm^{-1})				
							-0.506	-1.001	0.339	-0.193	-0.087
							-0.503	-0.070	-0.117	-1.384	-0.068
							-0.183	-3.170	0.621	0.127	2.311
							-0.438	0.176	0.276	-0.660	-0.436
							1.659	-0.569	-0.837	1.266	-0.564
							-0.257				
							-0.077	-0.144			
							1.749	-0.145	-0.184		
							-0.745	0.627	-0.315	-0.644	
							-2.398	-0.240	0.182	-0.125	-0.011
							-0.181	-0.765	-0.372	-0.416	0.022
							0.354	0.511	-0.096	-0.062	0.341
							-0.155	-0.425	-0.337	-1.289	-0.071
							-0.146	-0.959	0.121	6.536	-1.350
							0.100	-0.002	-0.331	-0.059	0.781
							0.111	0.950	0.621	-2.255	-1.064
							0.225				
							0.011	-0.125			
							0.761	-1.154	0.170		
							0.448	-0.375	0.067	-0.685	
							0.552	-0.261	1.696	0.365	0.559
							1.291	-0.383	-1.257	0.018	-0.317
							1.201				
CF_2O (C_{2v})	C	0.000000000	0.000000000	0.145592000	-312.803148	0.013912	Freqs.				
	O	0.000000000	0.000000000	1.316512000			1960.314				
	F	0.000000000	1.065245000	-0.633647000			962.534				
	F	0.000000000	-1.065245000	-0.633647000			576.081				
							775.952				
							1216.088				
							615.484				
							Anharm. coefficients				
							-10.999				
							10.151	-5.335			
							-1.002	-3.619	0.023		

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1}) and anharm. coefficients (cm^{-1})
							-5.967 -2.992 0.222 -0.184 -9.237 -11.979 -6.837 -6.126 -4.447 -6.312 -1.375 0.307 0.594 -4.232 0.125 (584; 626; 774; 965; 1249; 1928)[3]
CF_2OO (C_s)	C O O F F	-0.386094000 0.636644000 1.877520000 -1.545196000 -0.432220000	-0.028761000 -0.705486000 -0.000114000 -0.603249000 1.249623000	0.000056000 0.000007000 -0.000015000 -0.000024000 -0.000007000	-387.778377	0.016373	Freqs. 1704.952 1434.500 985.962 821.370 623.021 614.483 494.066 270.160 238.219 Anharm. coefficients -10.675 -5.474 -7.174 -12.539 -10.844 -1.923 2.809 -6.785 3.145 -6.376 -1.110 -8.244 -0.598 -3.194 -0.573 -17.450 -6.390 -4.828 1.823 1.735 -1.593 -5.962 -0.045 -3.290 -0.464 -1.112 -2.176 -1.106 -2.177 -1.445 -0.860 -1.600 -0.150 -5.901 -0.550 -2.689 -0.675 0.175 0.758 -0.556 0.279 1.820 3.611 0.526 -1.824

Table S2: High-pressure rate constants, $k^{\infty}(T)$, for the C_2F_4 + O_3 system calculated at CCSD(T)/CBS//B3LYP/aug-cc-pVTZ method[a].

No.	Reaction	$k(T) = A \times T^n \times \exp(-E_a/RT)$			$k^{\infty}(T)$ at 298 K [b]
		A [b]	n	E_a/R (K)	
1	$C_2F_4 + O_3 \rightarrow$ Adduct	4.80×10^{-23}	2.69	2.98×10^{3}	1.03×10^{-20}
	(reverse reaction)	2.27×10^{11}	0.95	4.70×10^{4}	1.60×10^{-55}
2	Adduct $\rightarrow CF_2O + CF_2OO$	1.25×10^{10}	1.31	1.36×10^{4}	3.57×10^{-7}
	(reverse reaction)	1.05×10^{-25}	3.31	1.32×10^{4}	8.69×10^{-37}

[a] Rate constants are valid for 200−1000 K. [b] Units of [s^{-1}] for first-order reactions and [cm^3 $molecule^{-1}$ s^{-1}] for second-order reactions. This work calculated at CCSD(T)/CBS//B3LYP/aug-cc-pVTZ method including Eckart tunneling, anharmonicity treatments and symmetry reactions.

Table S3: The calculated rate constants, $k^{\infty}(T)$, for the addition process, $C_2F_4 + O_3 \rightarrow$ Adduct (via TS1), over the range of temperature 200 – 1000 K, including the anharmonic, Eckart quantum tunneling treatments. Units are in cm^3/molecule/s.

T (K)	**$C_2F_4 + O_3 \rightarrow$ Adduct (via TS1)**		
	$k^{\infty}(T)$ (cm^3/molecule/s)	Anharmonic factor	Tunneling coefficient
200	2.49E-23	0.59	1.27
298	1.03E-20	0.50	1.11
300	1.12E-20	0.50	1.11
400	2.87E-19	0.43	1.06
500	2.28E-18	0.39	1.04
600	9.96E-18	0.35	1.03
700	3.07E-17	0.33	1.02
800	7.56E-17	0.32	1.02
900	1.60E-16	0.31	1.01
1000	3.01E-16	0.30	1.01

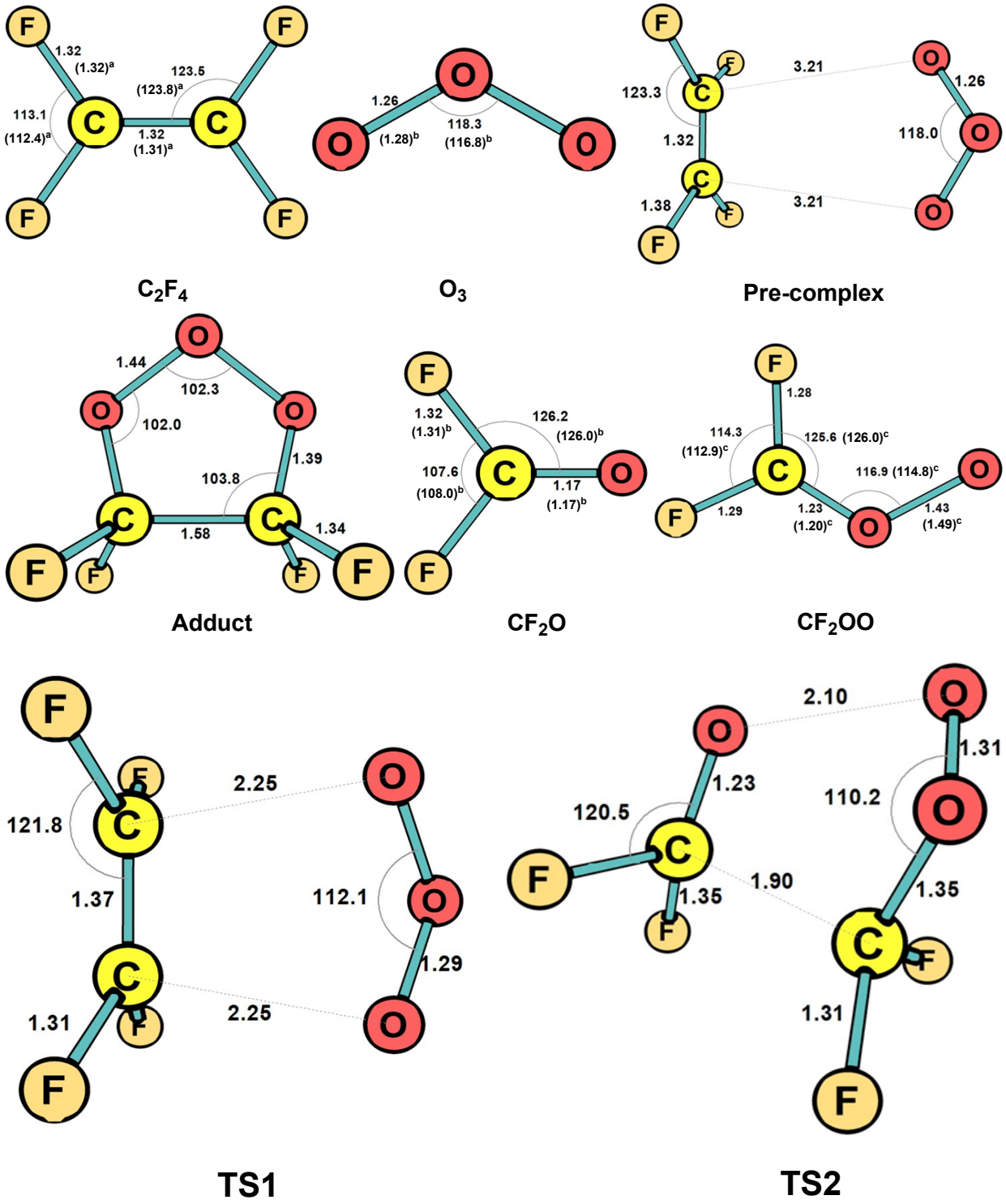

Figure S1: B3LYP/aug-cc-pVTZ optimized geometries for the species involved in the $C_2F_4 + O_3$ reaction. All structures were obtained for the lowest-energy conformer of a given species. Bond lengths are in Å and angles are in degree (°). [a] From the work of Hellwege *et al.*[4]; [b] from the work of Herzberg[1] and [c] from the work of Li *et al.*[5].

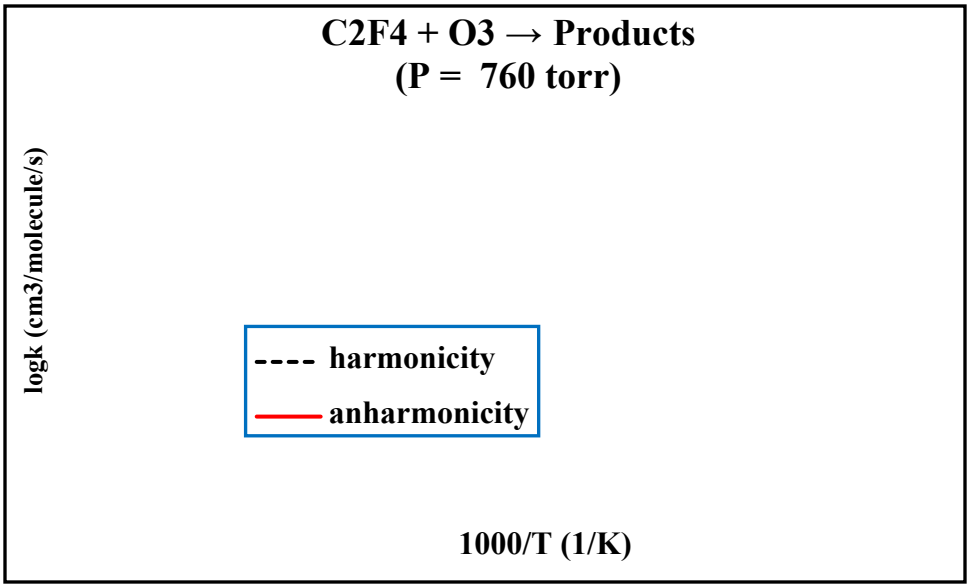

Figure S2: Comparison of the calculated rate coefficients obtained from the anharmonicity and harmonicity treatments for the $C_2F_4 + O_3 \rightarrow$ products reaction as a function of temperature at P = 760 torr.

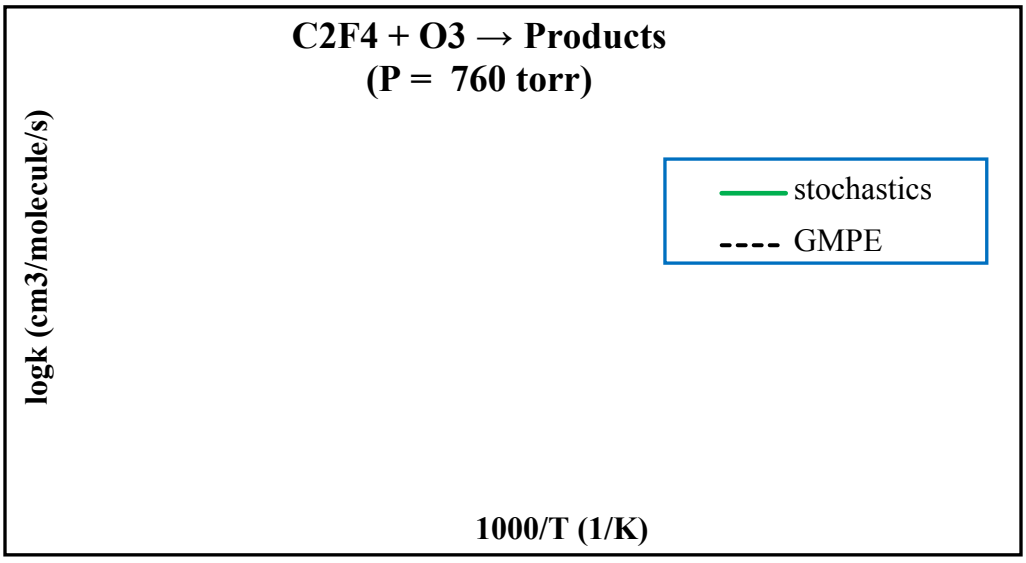

Figure S3: Comparison of the calculated coefficients obtained from the stochastic (solid line) and deterministic (dashed line) models as a function of temperature at P = 760 torr for the $C_2F_4 + O_3 \rightarrow$ products reaction.

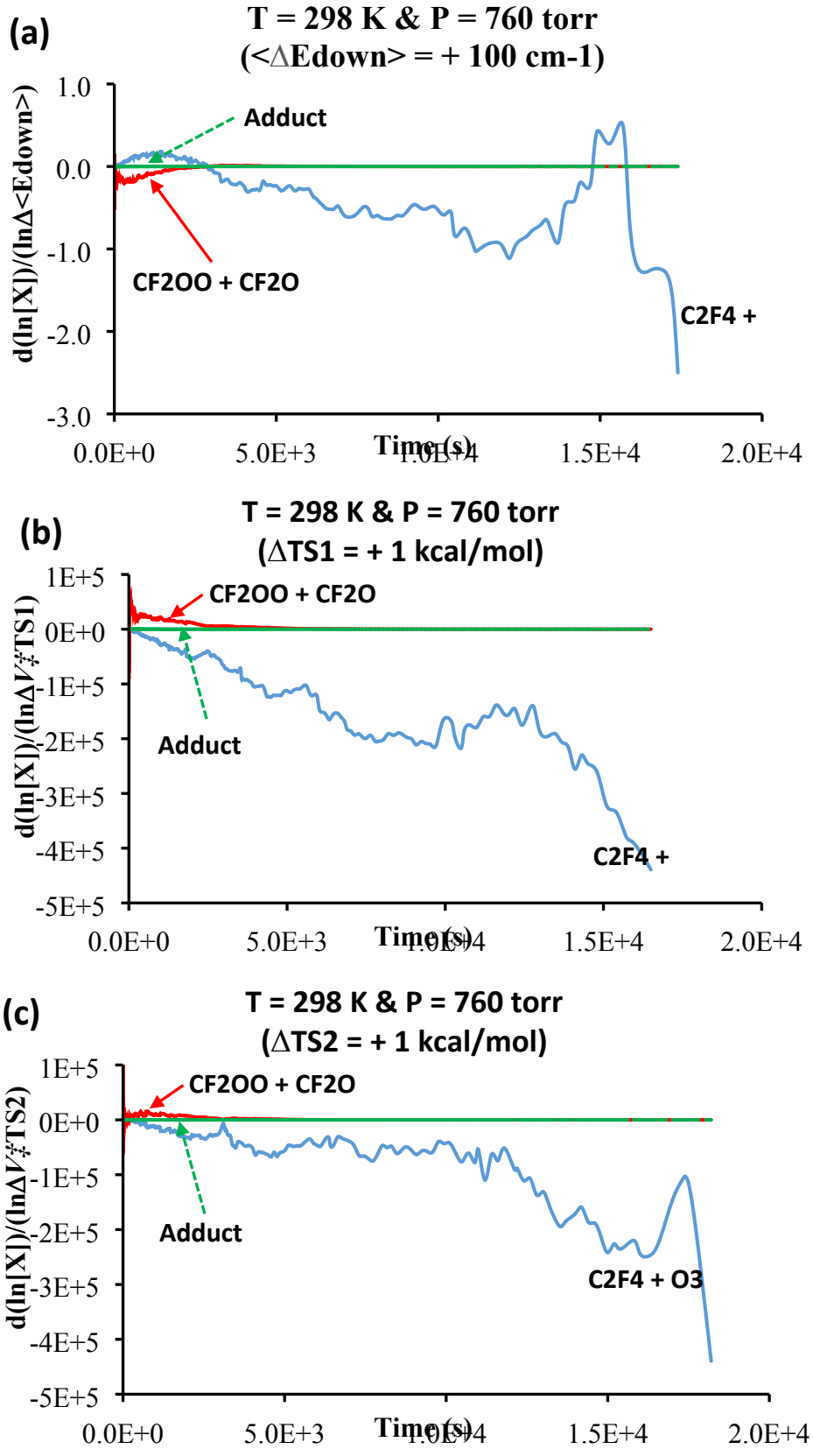

Figure S4: Normalized sensitivity coefficients for the species mole fraction [X] with respect to the energy transfer $<\Delta E_{down}>$= +100 cm^{-1} (a) and the barrier height $\Delta V^{\ddagger}$ of the TS1 & TS2 channels (b-c).

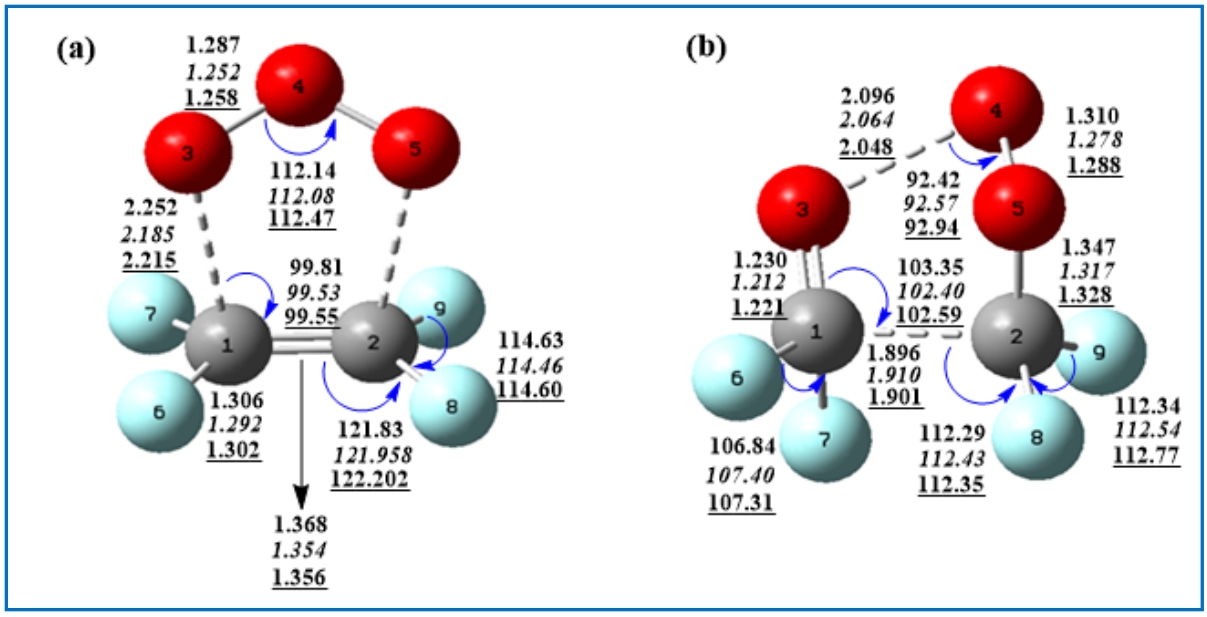

Figure S5: Geometrical structures of TS1 (a) and TS2 (b), optimized at B3LYP, BH&HLYP[6,7] (*italic*) and M06-2X[8] (underlined) with the same basis set, aug-cc-pVTZ. Bond lengths and angles are in Å and degrees (°), respectively.

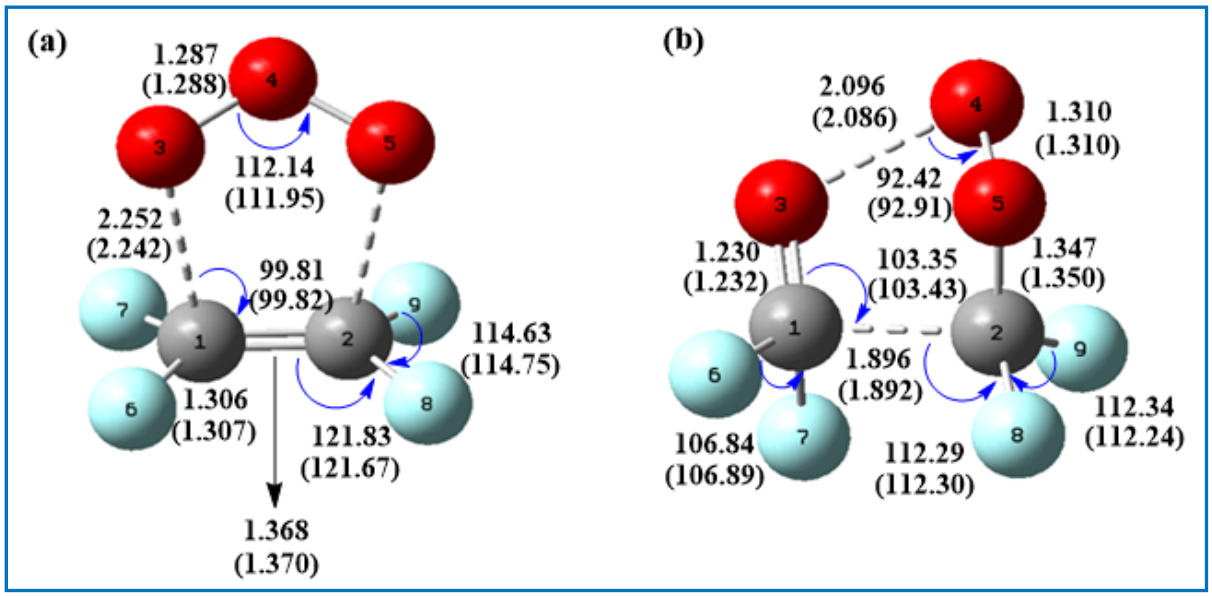

Figure S6: Geometrical structures of TS1 (a) and TS2 (b), optimized at B3LYP/aug-cc-pVTZ and B3LYP-D3/aug-cc-pVTZ (values given in parentheses). Bond lengths and angles are in Å and degrees (°), respectively.

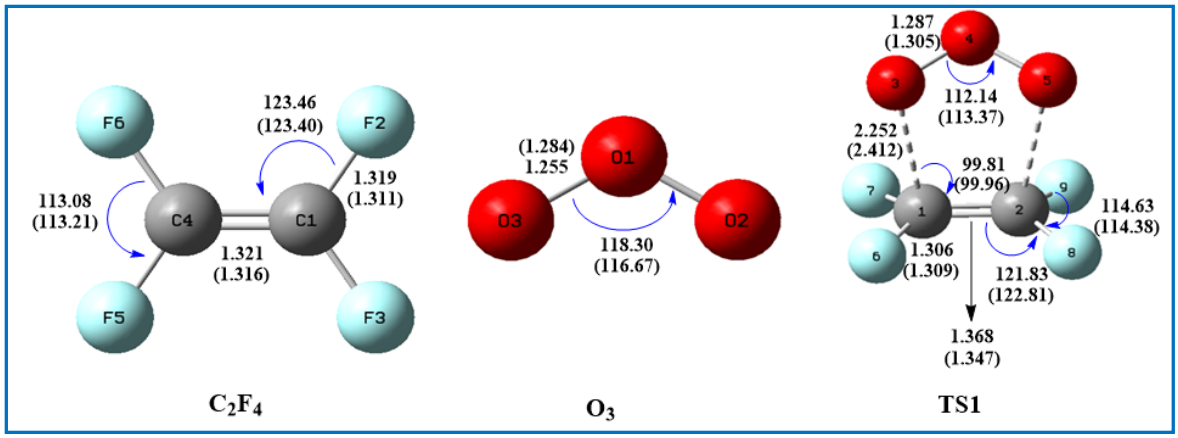

Figure S7: Geometrical structure of reactants & TS1 optimized at B3LYP/aug-cc-pVTZ and MP2/aug-cc-pVTZ (values given in parentheses). Bond lengths and angles are in Å and degrees (°), respectively.

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