

S1. Table of NMR chemical shifts for 37 fluorine-containing molecules in the gas phase, and adsorbed on 6 surfaces.

Reporter	#	δ_{Gas}	δ_{C18}	δ_{C8}	δ_{ACN}	δ_{SiO2}	δ_{Alu}	δ_{SiPP}	$\Delta\delta_{\text{C18}}$	$\Delta\delta_{\text{C8}}$	$\Delta\delta_{\text{ACN}}$	$\Delta\delta_{\text{SiO2}}$	$\Delta\delta_{\text{Alu}}$	$\Delta\delta_{\text{SiPP}}$
C6H5F	1	-122.40	-115.85	-117.92	-122.50	-120.09	-120.51	-120.01	6.55	4.48	-0.10	2.31	1.89	2.39
1,4-C6H4F2	2	-129.66	-122.54	-124.55	-131.26	-126.63	-125.84	-125.00	7.12	5.11	-1.60	3.03	3.82	4.66
1,2-C6F2H4	3	-147.50	-141.00	-143.33	-150.73	-146.20	-146.01	-146.00	6.50	4.17	-3.23	1.30	1.49	1.50
1,3,5-C6H3F3	4	-117.16	-110.57	-112.46	-117.65	-114.66	-	-112.56	6.59	4.70	-0.49	2.50	-	4.60
1,2,3-C6H3F3	5	-144.56	-138.09	-140.22	-148.08	-143.33	-142.72	-142.30	6.47	4.34	-3.52	1.23	1.84	2.26
		-170.73	-164.68	-167.15	-175.02	-170.44	-169.85	-170.30	6.05	3.58	-4.29	0.29	0.88	0.43
1,2,4,5-C6H2F4	6	-149.31	-142.61	-144.50	-150.92	-146.70	-145.90	-144.90	6.70	4.81	-1.61	2.61	3.46	4.41
C6F5H	7	-149.37	-141.91	-143.62	-149.56	-145.62	-145.51	-142.96	7.46	5.75	-0.19	3.75	3.86	6.41
		-163.99	-157.40	-160.17	-166.94	-162.87	-163.23	-162.55	6.59	3.82	-2.95	1.12	0.76	1.44
		-172.85	-165.79	-168.15	-174.22	-170.50	-170.62	-169.70	7.06	4.70	-1.37	2.35	2.23	3.15
C6F6	8	-173.26	-166.44	-168.45	-174.39	-169.50	-169.86	-169.07	6.82	4.81	-1.13	3.76	3.40	4.19
2Cl-C6H4F	9	-123.67	-117.91	-119.62	-127.01	-122.50	-122.42	-	5.76	4.05	-3.34	1.17	1.25	-
3Cl-C6H4F	10	-120.97	-113.68	-115.63	-121.79	-117.98	-117.63	-117.16	7.29	5.34	-0.82	2.99	3.34	3.81
4l-C6H4F	11	-124.84	-117.03	-118.90	-124.49	-121.38	-121.25	-119.49	7.81	5.94	0.35	3.46	3.59	5.35
2F-C6H4N	12	-75.32	-70.78	-71.50	-78.78	-77.02	-75.67	-75.12	4.54	3.82	-3.46	-1.70	-0.35	0.20
3F-C6H4N	13	-137.75	-128.17	-130.42	-137.64	-132.65	-133.48	-133.63	9.58	7.33	0.11	5.10	4.27	4.12
C5F5N	14	-95.44	-89.80	-91.51	-97.50	-93.92	-93.74	-93.26	5.64	3.93	-2.06	1.52	1.70	2.18
		-145.68	-137.21	-139.87	-146.03	-138.81	-138.34	-139.26	8.47	5.81	-0.35	6.87	7.34	6.42
		-172.67	-164.85	-167.21	-172.90	-167.68	-167.21	-167.31	7.82	5.46	-0.23	4.99	5.46	5.36
CH3-C6F5	15	-154.36	-146.95	-148.90	-155.12	-150.55	-150.19	-148.48	7.41	5.46	-0.76	3.81	4.17	5.88
		-169.15	-162.68	-165.10	-171.67	-167.98	-167.21	-168.00	6.47	4.05	-2.52	1.17	1.94	1.15
		-174.25	-167.32	-169.62	-176.25	-172.20	-171.26	-171.30	6.93	4.63	-2.00	2.05	2.99	2.95
2CH3-C6H4F	16	-127.07	-120.60	-122.55	-129.60	-124.20	-124.08	-124.15	6.47	4.52	-2.53	2.87	2.99	2.92
		δ_{Gas}	δ_{C18}	δ_{C8}	δ_{ACN}	δ_{SiO2}	δ_{Alu}	δ_{SiPP}	$\Delta\delta_{\text{C18}}$	$\Delta\delta_{\text{C8}}$	$\Delta\delta_{\text{ACN}}$	$\Delta\delta_{\text{SiO2}}$	$\Delta\delta_{\text{Alu}}$	$\Delta\delta_{\text{SiPP}}$
3CH3-C6H4F	17	-123.55	-116.91	-118.80	-125.08	-120.68	-120.79	-120.35	6.64	4.75	-1.53	2.87	2.76	3.20
2CF3-C6H4F	18	-121.32	-117.26	-118.80	-125.98	-121.46	-121.91	-120.70	4.06	2.52	-4.66	-0.14	-0.59	0.62
		-70.80	-65.38	-67.16	-73.55	-67.28	-67.10	-67.67	5.42	3.64	-2.75	3.52	3.70	3.13
3CF3-C6H4F	19	-120.38	-113.90	-115.63	-121.03	-118.09	-118.21	-116.90	6.48	4.75	-0.65	2.29	2.17	3.48
		-72.56	-66.61	-68.98	-75.55	-69.15	-68.68	-69.15	5.95	3.58	-2.99	3.41	3.88	3.41
CF3-C6F5	20	-148.61	-143.67	-145.15	-152.01	-146.58	-147.08	-145.66	4.94	3.46	-3.40	2.03	1.53	2.95
		-159.00	-151.41	-153.07	-159.06	-153.15	-152.72	-158.75	7.59	5.93	-0.06	5.85	6.28	0.25
		-171.09	-164.15	-165.75	-171.85	-166.53	-165.92	-	6.94	5.34	-0.76	4.56	5.17	-
		-64.41	-60.40	-61.58	-68.45	-61.84	-61.23	-61.27	4.01	2.83	-4.04	2.57	3.18	3.14
CF3-C6H5	21	-72.50	-66.91	-68.74	-75.38	-68.80	-	-	5.59	3.76	-2.88	3.70	-	-
4CF3-C6H4Cl	22	-72.44	-66.73	-68.33	-75.08	-68.68	-	-	5.71	4.11	-2.64	3.76	-	-
2CF3-C6H4Cl	23	-72.03	-66.32	-67.92	-74.55	-68.39	-67.97	-68.73	5.71	4.11	-2.52	3.64	4.06	3.30
4CF3-C6H4Br	24	-72.79	-67.26	-67.26	-74.67	-68.92	-68.26	-	5.53	5.53	-1.88	3.87	4.53	-
CF3CCl3	25	-89.99	-86.10	-87.29	-94.46	-87.70	-87.81	-87.41	3.89	2.70	-4.47	2.29	2.18	-
CFCl3	26	-8.10	-	-4.72	-10.49	-5.33	-6.08	-5.09	-	3.38	-2.38	2.77	2.02	3.01
CF2Br2	27	-0.75	3.42	1.91	-5.01	0.80	-1.82	-	4.17	2.66	-4.26	1.55	-1.07	-
C6F14	28	-88.99	-86.45	-86.82	-93.80	-86.37	-86.59	-86.63	2.54	2.17	-4.81	2.62	2.40	2.36
		-129.19	-127.47	-127.78	-134.82	-127.27	-127.61	-127.70	1.72	1.41	-5.63	1.92	1.58	1.49
		-133.12	-131.05	-131.36	-	-130.85	-131.07	-131.28	2.07	1.76	-	2.27	2.05	1.84
C9F20	29	-88.99	-86.16	-86.46	-93.65	-86.37	-86.47	-86.45	2.83	2.53	-4.66	2.62	2.52	2.54
		-128.07	-126.12	-126.37	-	-126.16	-126.32	-126.47	1.95	1.70	-	1.91	1.75	1.60
		-129.01	-127.00	-127.25	-134.26	-127.10	-127.20	-127.35	2.01	1.76	-5.25	1.91	1.81	1.66
		-133.06	-130.76	-131.06	-138.20	-130.85	-130.90	-131.11	2.30	2.00	-5.14	2.21	2.16	1.95
		δ_{Gas}	δ_{C18}	δ_{C8}	δ_{ACN}	δ_{SiO2}	δ_{Alu}	δ_{SiPP}	$\Delta\delta_{\text{C18}}$	$\Delta\delta_{\text{C8}}$	$\Delta\delta_{\text{ACN}}$	$\Delta\delta_{\text{SiO2}}$	$\Delta\delta_{\text{Alu}}$	$\Delta\delta_{\text{SiPP}}$
CF3-C6F11	30	-76.96	-74.48	-74.85	-	-74.96	-74.61	-74.83	2.48	2.11	-	2.00	2.35	2.13
		-126.02	-124.13	-124.43	-	-124.43	-124.26	-124.48	1.89	1.59	-	1.59	1.76	1.54
		-126.78	-124.84	-125.25	-	-125.20	-125.02	-125.24	1.94	1.53	-	1.58	1.76	1.54
		-129.07	-126.77	-127.13	-	-127.25	-126.78	-127.18	2.30	1.94	-	1.82	2.29	1.89
		-129.83	-127.53	-127.89	-	-128.01	-127.54	-127.94	2.30	1.94	-	1.82	2.29	1.89
		-130.71	-128.41	-128.78	-	-128.83	-128.60	-128.76	2.30	1.93	-	1.88	2.11	1.95
		-131.47	-129.17	-129.60	-	-129.66	-129.36	-129.52	2.30	1.87	-	1.81	2.11	1.95
		-138.96	-136.21	-136.64	-	-136.70	-136.40	-136.62	2.75	2.32	-	2.26	2.56	2.34
		-139.46	-137.04	-137.40	-	-137.52	-137.17	-137.39	2.42	2.06	-	1.94	2.29	2.07
		-147.67	-144.72	-145.15	-	-145.27	-144.97	-145.07	2.95	2.52	-	2.40	2.70	2.60
		-148.43	-145.49	-145.91	-	-146.03	-145.73	-145.84	2.94	2.52	-	2.40	2.70	2.59
		-149.73	-146.78	-147.14	-	-147.26	-147.08	-147.07	2.95	2.59	-	2.47	2.65	2.66
(CF3)2CHOH	31	-85.06	-78.88	-80.95	-87.34	-81.62	-83.06	-81.40	6.18	4.11	-2.28	3.44	2.00	3.66
CF3CH2OH	32	-87.98	-79.70	-82.12	-88.87	-83.85	-86.24	-83.05	8.28	5.86	-0.89	4.13	1.74	4.93
CF3COOH	33	-84.53	-79.17	-81.54	-88.01	-82.44	-83.65	-81.87	5.36	2.99	-3.48	2.09	0.88	2.66
C2F5COOH	34	-91.69	-86.86	-89.05	-96.68	-89.81	-89.46	-89.91	4.83	2.64	-4.99	1.88	2.23	1.78
		-130.18	-125.06	-127.07	-134.35	-127.84	-128.42	-125.83	5.12	3.11	-4.17	2.34	1.76	4.35
C6H11F	35	-229.63	-221.21	-223.67	-228.91	-219.12	-218.33	-223.40	8.42	5.96	0.72	10.51	11.30	6.23
C6H13F	36	-229.42	-219.68	-223.34	-228.12	-218.89	-218.92	-223.30	9.74	6.08	1.30	10.53	10.49	6.12
C7H15F	37	-228.28	-219.70	-221.33	-226.79	-219.35	-218.73	-222.36	8.58	6.95	1.49	8.93	9.55	5.92

