Zero-point vibrational contributions to fluorine shieldings in organic molecules: Supplementary material

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TABLE I. Contributions to the proton and carbon isotropic shielding constants of **fluoromethanes** as obtained at the Hartree–Fock level. All shielding constants reported in ppm.

		σ_e	σ_{eff}	σ_{eff} - σ_e	$\langle\sigma_2^{(0)}\rangle$	$\langle\sigma\rangle_{\rm ZPV}$	$\langle\sigma\rangle$
fluoromethane	σ^C	131.29	129.31	-1.98	-1.74	-3.72	127.57
	σ^H	28.51	28.21	-0.30	-0.32	-0.62	27.89
difluoromethane	σ^C	98.71	97.15	-1.56	-1.57	-3.13	95.58
	σ^H	27.60	27.34	-0.26	-0.34	-0.60	27.00
trifluoromethane	σ^C	90.83	89.61	-1.21	-0.84	-2.05	88.76
	σ^H	27.24	26.97	-0.27	-0.31	-0.58	26.66
tetrafluoromethane	σ^C	87.00	86.07	-0.93	-0.04	-0.97	86.03

TABLE II. Contributions to the proton and carbon isotropic shielding constants of **fluoroethanes** as obtained at the Hartree–Fock level. All shielding constants reported in ppm.

		σ_e	σ_{eff}	σ_{eff} - σ_e	$\langle\sigma_2^{(0)}\rangle$	$\langle\sigma\rangle_{\rm ZPV}$	$\langle\sigma\rangle$
fluoroethane[a]	σ^{C_1}	178.58	178.11	-0.47	-3.32	-3.79	174.79
	σ^{C_2}	123.39	121.77	-1.62	-2.65	-4.27	119.12
	$\sigma^{H_{1,2}}$	30.99	30.92	-0.07	-0.56	-0.63	30.36
	$\sigma^{H_{3,4}}$	28.41	28.17	-0.24	-0.40	-0.64	27.77
	σ^{H_5}	31.66	31.64	-0.02	-0.64	-0.66	31.00
1,2-difluoroethane[b]	σ^C	120.05	118.80	-1.25	-2.87	-4.12	115.93
	σ^{H_1}	28.13	27.95	-0.18	-0.41	-0.59	28.54
	σ^{H_2}	28.69	28.52	-0.17	-0.42	-0.59	28.10
1,1-difluoroethane[c]	σ^{C_1}	174.58	174.48	-0.10	-3.57	-3.67	170.91
	σ^{C_2}	92.54	91.09	-1.45	-1.77	-3.22	89.32
	$\sigma^{H_{1,2}}$	31.23	31.25	0.02	-0.64	-0.62	30.61
	σ^{H_3}	30.87	30.89	0.02	-0.62	-0.60	30.27
	σ^{H_4}	27.40	27.16	-0.24	-0.33	-0.57	26.83
1,1,1-trifluoroethane[d]	σ^{C_1}	174.42	174.45	0.03	-3.39	-3.36	171.06
	σ^{C_2}	82.31	81.18	-1.13	-0.86	-1.99	80.32
	$\sigma^{H_{1,2,3}}$	30.93	30.98	0.05	-0.63	-0.58	30.35
hexafluoroethane	σ^C	91.02	90.31	-0.72	-0.43	-1.15	89.87

[a] Connectivity: $H_5H_{1,2}$-C_1-C_2-$H_{3,4}F$
[b] The gauche conformation is studied (with H_1 closest to the F atom on the opposite group)
[c] Connectivity: (H_3 $H_{1,2}$)-C_1-C_2-($F_{1,2}$ H_4)
[d] Connectivity: ($H_{1,2,3}$)-C_1-C_2-($F_{1,2,3}$)

TABLE III. Contributions to proton and carbon the isotropic shielding constants of **fluoropropanes** as obtained at the Hartree–Fock level. All shielding constants reported in ppm.

		σ_e	σ_{eff}	σ_{eff} - σ_e	$\langle\sigma_2^{(0)}\rangle$	$\langle\sigma\rangle_{\rm ZPV}$	$\langle\sigma\rangle$
1-fluoropropane[a]	σ^{C_1}	171.92	170.58	-1.34	-3.16	-4.50	167.42
	σ^{C_2}	118.12	117.05	-1.07	-3.66	-4.73	113.39
	σ^{C_3}	186.32	186.40	0.08	-4.19	-4.11	182.21
	$\sigma^{H_{1,3}}$	28.59	28.40	-0.19	-0.42	-0.61	27.99
	$\sigma^{H_{2,4}}$	31.83	31.85	0.02	-0.71	-0.69	31.14
	σ^{H_5}	31.37	31.42	0.05	-0.72	-0.67	30.70
	$\sigma^{H_{6,7}}$	30.84	30.63	-0.21	-0.49	-0.70	30.14
2-fluoropropane[b]	σ^{C_1}	117.79	116.18	-1.61	-3.16	-4.77	113.02
	σ^{C_2}	173.21	173.35	0.14	-4.65	-4.51	168.70
	σ^{H_1}	31.63	31.68	0.05	-0.75	-0.70	30.93
	σ^{H_3}	31.22	31.24	0.02	-0.68	-0.66	30.56
	σ^{H_6}	30.91	30.93	0.02	-0.68	-0.66	30.25
	σ^{H_7}	28.21	27.98	-0.23	-0.40	-0.63	27.58
2,2-difluoropropane[c]	σ^{C_1}	87.12	85.71	-1.41	-1.12	-2.53	84.59
	σ^{C_2}	171.12	171.32	0.20	-3.85	-3.65	167.47
	$\sigma^{H_{1,2,3,4}}$	31.24	31.29	0.05	-0.77	-0.72	30.52
	$\sigma^{H_{5,6}}$	30.78	30.83	0.05	-0.75	-0.70	30.08
1,1,1-trifluoropropane[d]	σ^{C_1}	167.97	160.20	-0.77	-3.37	-4.14	163.83
	σ^{C_2}	81.31	80.29	-1.02	-1.07	-2.09	79.22
	σ^{C_3}	188.02	188.62	0.60	-5.55	-4.95	183.07
	$\sigma^{H_{1,2}}$	31.32	31.47	0.15	-1.00	-0.85	30.47
	σ^{H_3}	31.50	31.63	0.13	-0.90	-0.77	30.73
	$\sigma^{H_{4,5}}$	30.82	30.69	-0.13	-0.50	-0.63	30.19

[a] Connectivity: ($H_{1,3}$ F)-C_2-C_1($H_{6,7}$)-C_3-($H_{2,4}$ H_5)
[b] Connectivity: (H_1 H_3 H_6)-C_2-C_1(H_7 F)-C_2-(H_1 H_3 H_6)
[c] Connectivity: ($H_{3,4,6}$)-C_2-C_1($F_{1,2}$)-C_2-($H_{1,2,5}$)
[d] Connectivity: ($F_1F_{2,3}$)-C_2-C_1($H_{4,5}$)-C_3-($H_{1,2}H_3$)

TABLE IV. Contributions to proton and carbon the isotropic shielding constants of **fluorobutanes** as obtained at the Hartree–Fock level. All shielding constants reported in ppm.

		σ_e	σ_{eff}	σ_{eff} - σ_e	$\langle\sigma_2^{(0)}\rangle$	$\langle\sigma\rangle_{\rm ZPV}$	$\langle\sigma\rangle$
1-fluorobutane[a]	σ^{C_1}	177.72	176.78	-0.94	-3.90	-4.84	172.88
	σ^{C_2}	163.89	162.90	-0.99	-3.84	-4.83	159.06
	σ^{C_3}	180.46	180.98	0.52	-5.49	-4.97	175.49
	σ^{C_4}	118.96	118.21	-0.75	-3.94	-4.69	114.27
	$\sigma^{H_{1,2}}$	31.54	31.62	0.08	-0.81	-0.73	30.81
	$\sigma^{H_{3,4}}$	28.58	28.45	-0.13	-0.45	-0.58	28.00
	σ^{H_5}	31.34	31.43	0.09	-0.76	-0.67	30.67
	$\sigma^{H_{7,8}}$	31.53	31.37	-0.16	-0.59	-0.75	30.78
	$\sigma^{H_{9,10}}$	30.92	30.74	-0.18	-0.51	-0.69	30.23
2-fluorobutane[b]	σ^{C_1}	165.84	165.10	-0.74	-4.76	-5.50	160.34
	σ^{C_2}	113.38	111.89	-1.49	-3.04	-4.53	108.85
	σ^{C_3}	183.70	184.32	0.62	-6.65	-6.03	177.67
	σ^{C_4}	173.73	173.98	0.25	-5.04	-4.79	168.94
	σ^{H_1}	31.64	31.77	0.13	-1.16	-1.03	30.61
	σ^{H_2}	31.03	31.17	0.14	-1.12	-0.98	30.05
	σ^{H_3}	31.66	31.72	0.06	-0.85	-0.79	30.87
	σ^{H_4}	31.23	31.28	0.05	-0.80	-0.75	30.48
	σ^{H_5}	31.49	31.60	0.11	-1.06	-0.95	30.54
	σ^{H_6}	30.94	30.99	0.05	-0.72	-0.67	30.27
	σ^{H_7}	31.39	31.27	-0.12	-0.61	-0.73	30.66
	σ^{H_8}	31.04	30.90	-0.14	-0.54	-0.68	30.36
	σ^{H_9}	28.47	28.25	-0.22	-0.43	-0.65	27.82

[a] Connectivity: $(F_1H_{3,4})$-C_4-$C_2(H_{9,10})$-$C_1(H_{7,8})$-C_3-$(H_{1,2}H_5)$
[b] Connectivity: $(H_3H_4H_6)$-C_4-$C_2(H_9F_1)$-$C_1(H_7H_8)$-C_3-$(H_1H_2H_5)$

TABLE V. Contributions to proton and carbon the isotropic shielding constants of **fluoroethenes** as obtained at the Hartree–Fock level. All shielding constants reported in ppm.

		σ_e	σ_{eff}	σ_{eff} - σ_e	$\langle\sigma_2^{(0)}\rangle$	$\langle\sigma\rangle_{\rm ZPV}$	$\langle\sigma\rangle$
fluoroethene[a]	σ^{C_1}	95.46	94.16	-1.30	-2.91	-4.21	91.25
	σ^{C_2}	35.99	34.76	-1.23	-1.96	-3.19	32.80
	$\sigma^{H_{trans}}$	27.91	27.80	-0.11	-0.33	-0.44	27.47
	$\sigma^{H_{cis}}$	27.41	27.26	-0.15	-0.37	-0.52	26.89
	σ^{H_3}	25.96	25.79	-0.17	-0.30	-0.47	25.49
1,1-difluoroethene[b]	σ^{C_1}	129.16	128.15	-1.01	-2.44	-3.45	125.71
	σ^{C_2}	30.44	29.44	-1.00	-0.68	-1.68	28.76
	$\sigma^{H_{1,2}}$	28.57	28.49	-0.08	-0.39	-0.47	28.10
trans-1,2-difluoroethene	σ^{C}	46.95	45.66	-1.29	-2.27	-3.58	43.37
	σ^{H}	25.18	25.02	-0.16	-0.32	-0.48	24.70
cis-1,2-difluoroethene	σ^{C}	57.39	56.15	-1.24	-2.40	-3.64	53.75
	σ^{H}	26.52	26.38	-0.14	-0.31	-0.45	26.07
trifluoroethene[c]	σ^{C_1}	76.79	75.74	-1.05	-2.38	-3.43	73.36
	σ^{C_2}	37.12	36.07	-1.05	-1.35	-2.40	34.72
	σ^{H}	26.11	25.99	-0.12	-0.38	-0.50	25.61

[a] Connectivity: (H_{trans} H_{cis})-C_1=C_2(H_3 F)
[b] Connectivity: ($H_{1,2}$-C_1=C_2-$F_{1,2}$)
[c] Connectivity: (F_{trans} F_{cis})-C_2=C_1(F_3 H)

TABLE VI. Contributions to proton and carbon the isotropic shielding constants of **fluorobenzenes** as obtained at the Hartree–Fock level. All shielding constants reported in ppm.

		σ_e	σ_{eff}	σ_{eff} - σ_e	$\langle\sigma_2^{(0)}\rangle$	$\langle\sigma\rangle_{\rm ZPV}$	$\langle\sigma\rangle$
fluorobenzene	σ^{C_F}	25.66	24.49	-1.17	-3.70	-4.87	20.79
	σ^{C_o}	74.09	72.91	-1.18	-2.20	-3.38	70.71
	σ^{C_m}	56.32	55.09	-1.23	-2.27	-3.50	52.82
	σ^{C_p}	65.82	64.55	-1.27	-2.36	-3.63	62.19
	σ^{H_o}	25.11	24.99	-0.12	-0.28	-0.40	24.71
	σ^{H_m}	24.81	24.69	-0.12	-0.21	-0.33	24.48
	σ^{H_p}	25.15	25.04	-0.11	-0.19	-0.30	24.85
o-difluorobenzene	σ^{C_o}	70.60	69.47	-1.13	-1.70	-2.83	67.77
	σ^{C_F}	39.73	38.65	-1.08	-3.30	-4.38	35.35
	σ^{C_m}	63.78	62.56	-1.22	-1.95	-3.17	60.61
	σ^{H_o}	25.00	24.89	-0.11	-0.20	-0.31	24.69
	σ^{H_m}	25.15	25.04	-0.11	-0.15	-0.26	24.89
m-difluorobenzene	σ^{C_m}	53.64	52.47	-1.17	-2.92	-4.09	49.55
	$\sigma^{C_{2,3}}$	80.10	78.93	-1.17	-2.40	-3.57	76.53
	σ^{C_F}	24.04	22.94	-1.10	-2.85	-3.95	20.09
	σ^{C_o}	87.09	85.96	-1.13	-1.98	-3.11	83.98
	σ^{H_m}	24.81	24.69	-0.12	-0.19	-0.31	24.50
	$\sigma^{H_{2,3}}$	25.44	25.33	-0.11	-0.21	-0.32	25.12
	σ^{H_o}	25.38	25.27	-0.11	-0.27	-0.38	25.00
p-difluorobenzene	σ^{C_F}	31.25	30.09	-1.16	-1.72	-2.88	28.37
	σ^{C_H}	71.64	70.47	-1.17	-2.95	-4.12	67.52
	σ^{H}	25.13	25.01	-0.12	-0.32	-0.44	24.69