Computational NMR coupling constants: Shifting and scaling factors for evaluating $^1J_{CH}$ (Supporting Information)

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Table S1: Experimental and calculated $^1J_{CH}$ coupling constants[a] that involve sp^3 carbon.

Molecule	Exp.	(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)	(11)	(12)	(13)	(14)	(15)
1 CH_3-CH_3	124.90	111.90	119.18	116.25	119.99	118.74	121.21	122.43	131.52	128.48	132.43	130.89	130.85	132.25	132.92	132.21
2 CH_4	125.00	113.31	120.52	117.69	121.43	120.11	122.61	124.09	133.98	130.22	134.23	132.61	132.61	134.12	134.65	133.98
3 $CH_3C(O)C_6H_5$	125.70	113.54	121.30	117.94	121.73	120.35	122.88	124.44	134.57	130.59	134.58	133.02	132.89	134.34	135.08	134.38
4 CH_3COH	127.00	114.17	121.15	118.39	122.18	120.66	123.31	125.04	134.12	131.01	135.03	133.14	133.18	134.76	135.49	134.82
5 CH_3COOH	130.00	116.06	123.41	120.28	124.11	122.55	125.26	126.98	136.30	132.95	137.01	135.04	135.15	136.75	137.48	136.78
6 $\overline{C}H_3C(O)OCH_2CH_3$	130.30	115.55	122.87	119.74	123.55	122.09	124.73	126.42	135.62	132.35	136.39	134.60	134.62	136.13	136.89	136.19
7 $CH_2(COOH)_2$	132.00	117.09	124.44	121.17	125.06	123.38	126.20	128.45	136.42	134.26	138.34	136.16	136.32	137.89	138.89	138.13
8 $CH_3-C\equiv CH$	132.00	116.68	125.05	121.20	125.12	123.75	126.31	127.74	137.88	134.06	138.24	136.56	136.51	137.93	138.70	137.99
9 CH_3NH_2	133.00	117.31	124.44	121.83	125.79	124.03	126.92	128.64	138.30	134.97	139.21	136.43	137.09	138.78	139.58	138.94
10 $CH_3\overline{C}H_2(CN)$	135.50	118.69	126.17	123.03	127.05	125.65	128.27	129.76	139.48	135.90	140.13	138.34	138.41	139.85	140.66	139.89
11 $(CH_3)_2\overline{C}H(CN)$	135.50	118.19	125.62	122.52	126.53	125.18	127.77	129.06	138.23	135.10	139.28	137.37	137.60	138.97	139.86	139.06
12 $[(CH3)_2CH]_2\overline{C}H(OH)$	136.00	121.26	129.95	126.26	130.34	128.83	131.62	132.74	143.11	139.53	143.76	140.56	141.90	143.30	144.40	143.58
13 CH_3CN	136.10	120.20	128.08	124.53	128.56	127.08	129.74	131.56	141.66	137.74	142.04	140.25	140.22	141.71	142.51	141.78
14 $\overline{C}H_2[N(CH_3)_2]_2$	136.60	124.03	132.42	128.92	133.22	131.58	134.40	135.53	145.75	142.34	146.83	144.23	144.84	146.37	147.31	146.50
15 $(CH_3)_2N-C(O)H$	138.00	121.34	128.91	125.83	129.95	128.41	131.13	132.84	142.72	139.17	143.55	141.38	141.65	143.22	144.01	143.27
16 $\overline{C}H_2(OH)CH(CH_3)_2$	140.00	121.24	129.88	126.48	130.62	128.74	131.74	133.15	143.99	140.20	144.56	141.00	142.34	144.05	145.00	144.33
17 $(CH_3)_2O$	140.00	123.41	131.19	128.22	132.40	130.65	133.58	135.33	145.44	142.06	146.52	143.66	144.43	146.11	146.95	146.24
18 CH_3OH	141.00	123.45	131.21	128.21	132.43	130.37	133.50	135.48	145.46	142.17	146.68	143.16	144.28	146.12	147.00	146.38
19 $\overline{C}H(OH)(CH_3)C_6H_5$	142.50	125.63	133.97	130.34	134.63	132.64	135.80	137.34	146.36	143.85	148.33	144.43	145.91	147.67	148.82	148.06
20 $CH_3OC_6H_5$	143.00	126.38	134.68	131.25	135.54	133.93	136.77	138.39	148.83	145.23	149.79	147.31	147.82	149.41	150.27	149.51
21 $CH_2(CN)_2$	145.20	124.59	132.35	128.85	133.09	131.59	134.29	136.38	146.30	142.56	147.06	145.19	145.23	146.72	147.59	146.79
22 CH_3NO_2	146.70	129.06	136.71	133.29	137.62	135.58	138.77	141.41	151.29	147.60	152.23	149.54	149.87	151.70	152.68	151.95
23 $CH_2(OH)(CF_3)$	147.50	129.25	137.18	133.91	138.23	135.99	139.44	141.80	151.77	148.06	152.63	149.03	150.12	152.03	153.16	152.33
24 CH_3OCHO	147.00	130.55	138.59	135.15	139.58	137.78	140.78	142.87	153.28	149.51	154.22	151.52	152.07	153.80	154.69	153.92
25 CH_3F	149.10	131.20	138.79	136.00	140.47	138.24	141.55	143.87	154.57	150.72	155.51	151.63	152.97	154.92	155.83	155.19
26 $CH_2FC_6H_5$	151.00	132.12	140.63	137.31	141.80	139.94	143.08	144.97	155.53	151.78	156.53	153.19	154.20	156.08	157.11	156.29
27 $CH_2F(CN)$	166.00	140.75	149.12	145.57	150.45	148.31	151.64	154.15	164.82	160.79	165.96	162.31	163.52	165.35	166.44	165.60
28 $CH_2(NO_2)_2$	169.40	149.21	157.43	153.26	158.39	155.85	159.49	163.32	173.81	169.57	175.01	171.36	172.17	174.26	175.46	174.66
29 CH_2F_2	184.50	161.31	170.87	166.84	172.37	169.37	173.53	175.98	188.14	183.54	189.45	183.49	186.24	188.58	189.86	189.06
30 CHF_3	239.10	214.46	227.05	221.55	228.98	224.51	229.95	229.96	245.87	239.68	247.50	238.14	243.11	246.04	247.80	246.87

[a]See foodnote in Table S4 for label specification. The carbon involved in the coupling is indicated when necessary.

Table S1: Experimental and calculated $^{1}J_{CH}$ coupling constants[a] that involve sp^3 carbon (continuation).

	Molecule	(16)	(17)	(18)	(19)	(20)	(21)	(22)	(23)	(24)	(25)	(26)	(27)	(28)	(29)	(30)	(31)	(32)	(33)	(34)	(35)
1	CH_3-CH_3	111.95	120.46	118.03	121.69	120.05	121.51	113.13	119.48	116.76	121.36	118.67	120.08	152.90	150.92	152.50	147.56	151.97	157.08	122.45	120.98
2	CH_4	112.98	121.81	119.11	122.80	121.12	122.59	114.58	121.56	118.43	122.98	120.28	121.81	153.54	152.84	154.31	150.82	153.75	158.54	123.67	122.07
3	$CH_3C(O)C_6H_5$	113.88	123.02	119.93	123.61	121.90	123.48	114.37	121.61	117.95	122.55	119.74	121.28	153.79	152.74	154.46	149.57	153.84	158.59	124.46	122.97
4	CH_3COH	114.38	122.80	120.29	124.00	122.15	123.85	114.93	121.01	118.32	122.85	119.92	121.66	154.91	153.83	155.64	151.11	154.84	159.54	124.97	123.34
5	CH_3COOH	116.15	124.87	122.07	125.82	123.96	125.66	116.83	122.98	120.22	124.84	121.87	123.56	157.78	156.25	157.73	153.40	157.53	161.87	127.01	125.16
6	$\overline{C}H_3C(O)OCH_2CH_3$	115.69	124.41	121.58	125.31	123.50	125.17	116.36	122.59	119.72	124.34	121.44	123.11	157.16	155.79	157.31	152.89	156.88	161.31	126.51	124.67
7	$CH_2(COOH)_2$	117.75	124.29	123.45	127.22	125.22	127.12	117.75	122.52	120.71	125.50	122.28	124.06	159.05	157.72	159.22	154.44	159.00	163.30	129.06	126.69
8	$CH_3-C\equiv CH$	116.96	126.09	123.26	127.12	125.37	126.94	117.67	124.70	121.44	126.14	123.28	124.92	158.50	156.77	158.50	153.89	158.30	162.82	127.51	126.31
9	CH_3NH_2	117.65	126.77	124.00	127.91	125.86	127.64	119.21	125.92	122.90	127.73	124.57	126.34	161.32	159.14	160.32	155.88	160.18	164.89	128.85	127.35
10	$CH_3\overline{C}H_2(CN)$	119.23	128.30	125.36	129.28	127.53	129.14	119.59	125.92	122.90	127.81	124.85	126.46	162.08	160.00	161.99	156.91	161.66	166.17	129.88	128.43
11	$(CH_3)_2\overline{C}H(CN)$	118.92	127.46	124.98	128.85	127.14	128.74	119.09	125.71	122.21	127.30	124.32	125.72	162.24	159.85	162.28	156.29	161.65	166.69	129.45	128.03
12	$[(CH3)_2CH]_2\overline{C}H(OH)$	122.18	131.58	128.76	132.68	130.79	132.62	123.32	130.30	126.95	132.19	129.14	130.60	164.20	162.27	162.96	156.93	163.86	169.00	134.28	132.58
13	CH_3CN	120.46	129.52	126.62	130.58	128.74	130.41	121.06	126.87	124.49	129.29	126.30	128.02	163.12	161.68	163.29	159.32	163.25	167.23	131.26	129.72
14	$\overline{C}H_2[N(CH_3)_2]_2$	124.68	134.16	131.38	135.53	133.51	135.34	125.65	132.63	129.40	134.71	131.48	133.18	172.65	170.65	172.17	166.28	171.91	176.57	136.60	135.21
15	$(CH_3)_2N-C(O)H$	121.65	130.88	127.98	132.01	130.11	131.82	122.97	129.77	126.62	131.61	128.56	130.24	166.78	164.72	165.83	161.46	165.99	170.18	133.15	131.44
16	$\overline{C}H_2(OH)CH(CH_3)_2$	122.25	132.70	129.19	133.21	131.05	132.99	123.54	130.67	127.64	132.82	129.47	131.24	166.13	164.24	165.09	160.30	165.53	170.29	134.29	132.93
17	$(CH_3)_2O$	123.92	133.39	130.60	134.72	132.68	134.50	125.68	132.68	129.59	134.64	131.42	133.33	170.23	168.51	169.36	165.05	169.55	173.82	135.69	134.25
18	CH_3OH	124.01	133.41	130.68	134.84	132.58	134.54	125.94	132.86	129.77	134.88	131.40	133.42	170.34	168.26	168.90	164.92	169.24	173.35	135.97	134.43
19	$\overline{C}H(OH)(CH_3)C_6H_5$	126.53	135.04	132.98	137.12	134.78	136.93	127.53	134.12	130.92	136.29	132.75	134.65	171.38	167.82	168.86	163.10	169.65	174.24	138.52	136.83
20	$CH_3OC_6H_5$	126.84	136.60	133.62	137.84	135.89	137.64	128.40	135.93	132.35	137.56	134.37	136.20	174.57	172.91	173.62	169.38	174.07	177.78	138.75	137.27
21	$CH_2(CN)_2$	125.36	134.75	131.51	135.66	133.84	135.53	125.27	131.74	128.35	133.47	130.29	132.10	169.65	168.03	169.56	165.28	170.05	173.63	136.36	134.80
22	CH_3NO_2	129.65	138.74	135.78	140.02	137.76	139.86	130.74	136.60	133.80	139.02	135.37	137.56	178.72	177.51	178.60	174.16	178.64	182.08	142.32	139.58
23	$CH_2(OH)(CF_3)$	130.37	139.59	136.56	140.77	138.40	140.66	131.32	138.09	134.41	139.66	135.91	138.25	179.37	176.43	177.04	172.85	177.40	180.64	143.12	140.51
24	CH_3OCHO	130.99	140.64	137.61	141.94	139.86	141.75	132.72	139.61	136.29	141.64	138.23	140.22	180.63	178.92	179.42	175.72	179.91	183.19	143.34	141.44
25	CH_3F	131.88	141.89	138.68	143.10	140.76	142.81	134.25	141.58	138.01	143.43	139.71	141.90	181.61	179.80	179.78	176.58	180.85	183.75	144.50	142.66
26	$CH_2FC_6H_5$	133.50	143.31	140.25	144.64	142.40	144.53	134.78	142.09	138.31	143.85	140.31	142.37	182.13	179.12	179.42	175.51	180.86	183.88	146.10	144.28
27	$CH_2F(CN)$	142.10	152.01	148.71	153.47	151.17	153.29	143.36	150.22	146.38	152.23	148.38	150.71	194.69	192.06	192.62	188.92	193.97	195.99	155.19	152.90
28	$CH_2(NO_2)_2$	150.51	160.09	156.60	161.56	158.90	161.41	151.21	157.06	153.36	159.59	155.21	157.77	209.77	209.41	210.83	205.41	211.06	213.14	165.91	161.62
29	CH_2F_2	162.73	174.06	170.21	175.66	172.80	175.43	165.25	173.06	168.63	175.24	170.51	173.69	229.06	226.45	227.95	222.71	228.71	229.74	178.09	175.63
30	CHF_3	214.80	229.51	224.13	231.36	227.59	231.05	216.84	226.38	220.51	229.11	222.72	227.45	299.44	295.28	299.33	291.97	300.62	298.10	234.19	232.18

[a]See foodnote in Table S4 for label specification. The carbon involved in the coupling is indicated when necessary.

Table S2: Experimental and calculated ${}^{1}J_{CH}$ coupling constants[a] that involve sp^2 carbon.

Molecule	Exp.	(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)	(11)	(12)	(13)	(14)	(15)
31 $trans-CH(CH_3)=CH(CH_3)$	148.70	135.58	142.73	139.17	143.69	141.79	144.87	147.70	157.04	153.27	158.06	155.50	155.81	157.63	158.53	157.74
32 $HCH=C\overline{H}(CH_3)$	152.00	137.66	144.73	141.49	146.02	144.04	147.30	149.76	159.17	155.56	160.38	157.66	158.06	159.99	160.91	160.10
32 $\overline{H}_cCH=CH(CH_3)$	153.10	140.34	147.99	144.57	149.22	147.25	150.46	153.22	163.55	159.53	164.53	162.32	162.21	164.15	165.02	164.27
33 $\overline{H}_cCH=CH-CH=CH_2$	154.91	141.03	149.32	145.65	150.28	148.55	151.77	154.42	165.01	161.04	166.01	163.91	163.77	165.76	166.60	165.82
34 $CH_2=CH_2$	156.20	142.78	150.97	147.23	151.96	149.87	153.24	155.72	166.54	162.26	167.35	164.92	164.95	167.00	167.86	167.10
35 $\overline{H}_cCH=CH(CHO)$	156.60	142.19	150.23	146.82	151.58	149.64	152.81	155.09	165.90	161.86	166.98	164.56	164.66	166.60	167.43	166.71
32 $HC\overline{H}_t=CH(CH_3)$	157.00	144.06	151.98	148.55	153.27	151.14	154.54	157.07	167.70	163.60	168.69	166.23	166.20	168.28	169.20	168.46
36 $\overline{H}_cCH=FCH$	159.18	145.95	153.87	150.21	154.94	152.97	156.27	159.71	169.94	165.78	170.87	169.08	168.58	170.51	171.51	170.61
33 $HC\overline{H}_t=CH-CH=CH_2$	159.21	145.59	153.77	149.92	154.69	152.75	156.23	159.29	169.82	165.66	170.79	168.39	168.31	170.44	171.43	170.63
36 $HC\overline{H}_t=FCH$	162.16	148.55	156.92	153.36	158.34	155.43	159.27	161.89	172.56	168.52	173.86	170.28	170.62	173.11	174.07	173.53
35 $HC\overline{H}_t=CH(CHO)$	162.30	147.55	155.22	151.63	156.49	154.25	157.89	161.09	171.57	167.28	172.52	169.95	169.94	172.05	173.18	172.28
35 $HCH=C\overline{H}(CHO)$	162.30	149.20	156.74	152.72	157.61	155.24	158.88	162.57	172.64	168.20	173.43	170.06	170.72	172.88	174.01	173.13
37 $trans-HC(CH_3)=NOH$	163.00	142.32	151.05	147.21	151.94	149.25	153.10	157.21	168.14	164.11	169.22	165.23	166.28	168.54	169.73	168.94
38 $\overline{H}_cCH=CH(CN)$	163.20	149.20	157.62	153.80	158.80	156.79	160.05	162.46	173.67	169.32	174.68	172.33	172.32	174.28	175.16	174.39
38 $HC\overline{H}_t=CH(CN)$	165.43	149.17	157.46	153.53	158.51	156.22	159.82	162.51	173.35	169.05	174.41	171.69	171.77	173.90	174.96	174.13
39 $CH_2=C=CH_2$	168.20	153.76	162.06	158.28	163.38	161.05	164.52	167.72	178.29	174.48	179.98	177.40	177.27	179.45	180.42	179.69
40 $CH_2=O$	172.00	155.85	166.09	162.08	167.30	164.41	168.61	171.50	184.50	179.91	185.65	180.57	182.48	184.93	186.21	185.41
41 $HC(O)CH_3$	172.40	150.01	160.10	156.16	161.24	158.53	162.59	163.94	177.22	172.16	177.66	172.56	174.64	176.92	178.28	177.38
42 $HC(O)C_6H_5$	173.70	152.48	162.48	158.51	163.75	160.91	165.00	166.82	179.61	174.95	180.59	175.49	177.39	179.78	181.16	180.28
38 $HCH=C\overline{H}(CN)$	176.74	156.30	164.05	160.21	165.47	163.00	166.57	170.09	180.63	176.25	181.84	178.43	179.04	181.24	182.28	181.45
43 $cis-HC(CH_3)=NOH$	177.00	163.54	172.52	167.96	173.50	169.84	173.64	175.84	187.02	182.55	188.40	183.43	184.34	186.50	187.76	186.93
44 $cis-H(CN)C=CH(CN)$	184.00	160.57	168.74	164.31	169.70	167.15	170.87	175.05	185.14	181.04	186.80	183.15	183.91	186.08	187.30	186.41
45 $HC(O)NH_2$	188.30	168.55	180.18	175.76	181.48	177.28	182.38	183.61	198.12	193.26	199.46	192.37	194.94	198.07	199.70	199.08
46 $HC(O)N(CH_3)_2$	191.20	170.37	182.50	177.18	182.95	179.52	184.03	185.28	199.22	194.50	200.70	194.75	196.84	199.58	201.12	200.31
36 $HCH=C\overline{H}F$	200.20	177.75	188.48	183.90	190.06	186.20	190.89	193.86	207.53	202.29	208.88	202.60	204.66	207.71	208.96	208.41
47 $HCOO(CH_3)$	226.20	201.79	214.29	208.85	215.55	211.38	216.89	218.36	234.31	228.22	235.42	228.04	230.90	234.22	235.95	235.09
48 $HC(O)F$	267.00	230.70	245.72	239.34	247.13	241.76	248.01	250.19	269.12	261.78	270.20	260.86	264.70	268.61	270.42	269.76

[a] See foodnote in Table S4 for label specification. The hydrogen involved in the coupling is indicated when necessary.

Table S2: Experimental and calculated $^1J_{CH}$ coupling constants[a] that involve sp^2 carbon (continuation).

Molecule	(16)	(17)	(18)	(19)	(20)	(21)	(22)	(23)	(24)	(25)	(26)	(27)	(28)	(29)	(30)	(31)	(32)	(33)	(34)	(35)
31 $trans-CH(CH_3)=CH(CH_3)$	136.06	144.82	141.74	146.16	143.90	145.94	138.39	144.00	140.34	146.14	142.52	144.47	188.35	185.74	188.31	181.27	186.88	192.76	147.61	145.25
32 $HCH=C\overline{H}(CH_3)$	138.07	146.44	144.02	148.47	146.17	148.30	140.41	145.99	142.54	148.38	144.64	146.74	192.12	189.81	192.03	185.40	190.56	195.94	149.65	147.49
32 $\overline{H}_cCH=CH(CH_3)$	140.80	150.47	147.15	151.75	149.41	151.56	143.35	149.75	146.08	151.97	148.24	150.46	194.13	193.02	195.64	189.51	194.13	199.37	152.63	150.79
33 $\overline{H}_cCH=CH-CH=CH_2$	141.89	151.81	148.57	153.16	150.83	153.00	145.36	151.65	147.68	153.99	149.83	152.08	196.80	195.46	197.56	191.19	196.57	201.92	153.93	152.31
34 $CH_2=CH_2$	143.17	153.61	149.78	154.47	152.07	154.28	145.86	152.64	148.68	154.63	150.82	153.18	198.30	196.74	198.81	192.57	197.70	202.74	155.06	153.40
35 $\overline{H}_cCH=CH(CHO)$	142.38	152.52	149.20	153.92	151.53	153.65	145.44	152.13	148.35	154.38	150.57	152.81	198.53	197.41	198.61	193.28	198.30	202.92	154.46	152.93
32 $HC\overline{H}_t=CH(CH_3)$	144.53	154.54	151.13	155.80	153.37	155.65	146.88	153.47	149.69	155.65	151.79	154.20	198.79	196.92	199.57	192.63	198.16	203.35	156.40	154.76
36 $\overline{H}_cCH=FCH$	146.87	156.38	152.97	157.65	155.32	157.61	149.15	155.48	151.45	157.42	153.55	156.01	202.06	201.05	203.83	198.06	202.33	207.03	159.02	156.72
33 $HC\overline{H}_t=CH-CH=CH_2$	146.67	156.55	153.13	157.86	155.37	157.76	150.00	156.03	151.89	158.35	153.97	156.47	202.44	200.66	202.86	196.25	201.74	206.90	158.81	156.84
36 $HC\overline{H}_t=FCH$	149.11	159.01	155.67	160.59	157.50	160.20	151.04	157.75	153.73	159.84	155.31	158.24	202.83	201.07	203.99	198.00	202.54	207.50	161.43	159.45
35 $HC\overline{H}_t=CH(CHO)$	148.39	158.22	154.67	159.51	156.96	159.45	151.31	157.40	153.47	159.68	155.55	158.21	205.71	204.52	206.21	200.89	205.26	209.44	160.60	158.71
35 $HCH=C\overline{H}(CHO)$	149.97	159.28	155.58	160.38	157.73	160.31	152.07	157.39	153.60	159.75	155.53	158.17	209.11	206.33	207.78	200.91	206.98	211.55	161.67	159.24
37 $trans-HC(CH_3)=NOH$	144.47	154.42	151.31	155.99	153.19	155.85	146.99	154.13	149.96	156.05	151.74	154.34	198.74	199.07	200.83	193.68	200.08	204.66	158.09	155.60
38 $\overline{H}_cCH=CH(CN)$	149.60	160.15	156.53	161.48	159.06	161.24	152.79	159.41	155.53	161.89	157.85	160.21	209.61	209.38	211.00	205.47	210.21	214.20	161.71	160.41
38 $HC\overline{H}_t=CH(CN)$	149.81	159.98	156.44	161.38	158.79	161.23	152.88	159.13	155.33	161.62	157.44	160.06	208.41	207.02	208.68	202.67	208.06	212.31	161.98	160.37
39 $CH_2=C=CH_2$	154.63	164.58	161.40	166.46	163.79	166.24	156.01	162.62	158.72	165.02	160.93	163.51	208.09	206.85	210.48	203.85	208.78	214.08	166.88	165.29
40 $CH_2=O$	157.58	169.70	165.86	171.14	168.16	171.07	161.71	170.17	165.95	172.34	167.87	171.20	214.00	213.08	214.63	209.17	215.73	218.49	171.35	170.60
41 $HC(O)CH_3$	151.33	163.81	159.44	164.53	161.69	164.51	154.27	162.85	158.49	164.84	160.58	163.53	204.93	203.96	204.58	199.60	206.13	209.38	164.75	164.05
42 $HC(O)C_6H_5$	154.04	165.94	161.99	167.21	164.24	167.16	156.55	165.15	160.75	167.22	162.86	165.85	206.05	204.33	205.15	199.43	207.16	210.53	167.38	166.55
38 $HCH=C\overline{H}(CN)$	157.44	167.30	163.66	168.82	166.12	168.57	159.05	164.44	160.91	167.46	163.04	165.70	215.36	212.99	215.49	208.57	214.33	218.50	169.28	167.50
43 $cis-HC(CH_3)=NOH$	162.87	173.20	169.63	175.03	171.14	173.81	165.07	171.44	167.44	174.26	168.70	171.63	223.71	220.48	222.93	215.81	220.96	224.99	175.07	173.67
44 $cis-H(CN)C=CH(CN)$	162.17	171.74	168.27	173.57	170.79	173.36	163.97	169.52	165.42	172.15	167.61	170.38	222.50	219.78	221.81	214.72	221.38	225.20	174.56	172.51
45 $HC(O)NH_2$	169.87	183.28	179.17	184.88	180.88	184.61	171.68	181.08	176.83	183.77	178.16	182.29	226.88	224.59	226.72	221.94	227.97	230.44	184.67	184.41
46 $HC(O)N(CH_3)_2$	171.49	184.28	180.37	186.08	182.55	185.93	173.08	183.04	177.88	184.88	179.83	183.48	227.50	225.31	227.66	221.64	228.50	231.93	186.25	185.47
36 $HCH=C\overline{H}F$	179.54	192.25	187.83	193.92	190.04	193.36	182.02	190.39	185.38	193.02	187.25	190.92	245.80	245.28	246.06	240.39	245.79	248.24	195.79	193.75
47 $HCOO(CH_3)$	202.92	217.59	212.34	219.00	214.94	218.93	204.90	214.42	208.58	216.87	210.50	215.29	272.65	268.73	270.95	264.24	271.82	272.39	220.47	218.91
48 $HC(O)F$	232.66	250.06	243.65	251.46	246.65	251.09	234.27	245.83	238.94	248.14	240.95	246.56	307.02	305.01	306.77	300.54	308.87	306.52	254.30	252.28

[a]See foodnote in Table S4 for label specification. The hydrogen involved in the coupling is indicated when necessary.

Table S3: Experimental and calculated $^1J_{CH}$ coupling constants[a] that involve sp carbon.

Molecule		Exp.	(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)	(11)	(12)	(13)	(14)	(15)
49	$HC \equiv C(CH_2OH)$	248.00	240.17	253.17	246.05	254.32	250.06	255.30	258.56	275.35	267.69	276.51	271.23	271.88	275.37	276.77	275.94
8	$HC \equiv C(CH_3)$	248.00	238.57	252.03	244.53	252.77	248.78	253.76	256.73	273.49	265.92	274.68	269.89	270.32	273.66	274.96	274.12
50	$HC \equiv CH$	249.00	240.27	252.00	244.89	253.12	249.16	254.29	258.67	274.29	266.64	275.40	270.87	271.05	274.41	275.84	274.90
51	$HC \equiv C(C_6H_5)$	251.00	239.89	253.41	246.27	254.62	250.64	255.61	258.44	275.53	268.07	276.96	272.07	272.57	275.93	277.22	276.36
52	$HC \equiv C(CH_2CN)$	251.00	244.29	257.90	250.56	259.00	255.02	260.06	262.62	279.74	272.19	281.17	276.33	276.81	280.15	281.51	280.61
53	$HC \equiv CCH = CH_2$	251.70	240.78	253.81	246.59	254.94	250.94	255.94	259.48	276.64	268.61	277.50	272.64	273.10	276.44	277.78	276.90
54	$HC \equiv CC(CH_3)_2OH$	253.00	238.66	252.10	245.11	253.38	249.26	254.35	256.95	274.15	266.57	275.37	270.36	270.89	274.29	275.63	274.79
55	$HC \equiv CC \equiv CH$	259.00	246.67	260.23	252.80	261.44	257.49	262.47	265.83	283.65	275.35	284.56	279.54	280.19	283.52	284.84	283.92
56	$HC \equiv N$	269.00	244.18	256.48	248.87	257.42	252.81	258.34	268.11	285.06	276.38	285.67	280.62	280.76	284.70	286.04	285.42
57	$HC \equiv CF$	275.50	271.21	283.48	276.18	285.48	280.94	286.51	290.10	306.41	298.26	308.11	302.67	303.23	306.84	308.45	307.45

[a]See foodnote in Table S4 for label specification.

Table S3: Experimental and calculated $^1J_{CH}$ coupling constants[a] that involve sp carbon (continuation).

Molecule		(16)	(17)	(18)	(19)	(20)	(21)	(22)	(23)	(24)	(25)	(26)	(27)	(28)	(29)	(30)	(31)	(32)	(33)	(34)	(35)
49	$HC \equiv C(CH_2OH)$	240.31	255.30	248.91	257.06	252.73	256.67	242.53	251.12	244.50	254.65	247.96	252.71	326.98	324.63	321.41	315.37	321.99	323.02	257.20	255.01
8	$HC \equiv C(CH_3)$	238.65	253.78	247.31	255.40	251.31	255.02	240.76	250.47	242.98	253.13	246.63	251.18	323.75	323.41	321.20	316.45	320.21	320.43	255.25	253.25
50	$HC \equiv CH$	240.20	254.49	247.77	255.85	251.78	255.62	243.24	251.30	243.84	254.03	247.54	252.18	328.83	327.80	324.50	319.94	323.18	323.16	257.24	253.76
51	$HC \equiv C(C_6H_5)$	240.33	255.63	249.38	257.62	253.46	257.19	242.53	250.85	245.08	255.43	248.81	253.34	326.51	327.01	324.52	320.18	323.76	323.70	257.12	255.59
52	$HC \equiv C(CH_2CN)$	244.34	259.92	253.37	261.68	257.55	261.34	246.63	255.09	248.88	259.19	252.68	257.34	333.24	331.86	328.40	322.61	329.27	329.54	261.19	259.52
53	$HC \equiv CCH = CH_2$	241.14	256.79	249.78	258.01	253.85	257.58	243.73	253.46	245.59	255.96	249.35	253.86	326.64	325.66	322.90	317.27	323.07	323.80	258.09	255.96
54	$HC \equiv CC(CH_3)_2OH$	238.87	254.27	247.90	256.04	251.80	255.64	240.86	250.99	243.56	253.79	247.14	251.77	325.48	325.57	323.07	318.85	322.23	322.07	255.67	254.03
55	$HC \equiv CC \equiv CH$	247.22	263.40	256.23	264.78	260.61	264.30	250.23	259.79	252.15	262.95	256.21	260.72	337.45	338.78	336.06	331.56	335.07	335.09	264.55	262.76
56	$HC \equiv N$	247.42	262.61	255.10	263.62	259.04	263.43	249.51	258.07	249.56	260.29	253.19	258.23	331.96	334.54	327.50	326.59	328.23	325.74	267.20	262.34
57	$HC \equiv CF$	270.67	285.33	278.32	287.46	282.83	287.13	273.03	280.76	273.07	284.34	277.06	282.45	361.73	360.65	359.66	354.75	358.61	359.16	288.89	285.40

[a]See foodnote in Table S4 for label specification.

Table S4: Experimental and calculated $^1J_{CH}$ coupling constants[a] that involve *aromatic* carbon.

Molecule	Exp.	(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)	(11)	(12)	(13)	(14)	(15)
58 $(CH_3)_3C_6H_3$	154.00	141.07	147.96	144.16	148.86	146.81	149.95	153.15	162.12	158.15	163.09	160.01	160.69	162.65	163.52	162.78
59 $C_6H_5F(o)$	155.00	148.92	155.69	151.97	156.80	154.56	157.99	161.90	170.83	166.68	171.81	168.92	169.24	171.31	172.32	171.51
60 $C_6H_5NH_2(o)$	156.01	141.10	148.06	144.43	149.05	146.80	150.14	153.47	163.02	158.68	163.60	160.38	161.00	163.07	164.01	163.30
60 $C_6H_5NH_2(m)$	156.90	143.81	150.62	146.88	151.62	149.20	152.72	155.77	164.92	160.78	165.82	162.32	163.03	165.23	166.21	165.52
61 $(CH_3)_3C_5H_2N$	158.00	145.03	152.02	148.01	152.77	150.40	153.84	157.79	166.56	162.71	167.75	164.22	165.06	167.20	168.20	167.44
62 $C_6H_5OH(o)$	158.35	144.03	150.74	147.02	151.69	149.47	152.86	156.56	165.60	161.50	166.46	163.38	163.89	165.97	166.95	166.18
63 C_6H_6	158.50	145.57	152.50	148.66	153.43	151.17	154.61	157.61	166.80	162.68	167.76	164.52	165.11	167.24	168.21	167.46
62 $C_6H_5OH(m)$	158.99	145.21	151.95	148.22	152.99	150.59	154.14	157.29	166.39	162.25	167.32	163.88	164.57	166.75	167.76	167.01
64 $C_6H_5CHO(p)$	160.43	146.27	152.94	149.27	154.09	151.84	155.30	158.48	167.72	163.49	168.60	165.36	166.00	168.10	169.10	168.30
60 $C_6H_5NH_2(p)$	160.46	148.53	155.57	151.73	156.57	154.11	157.66	160.68	170.55	165.86	171.01	167.47	168.17	170.41	171.39	170.72
62 $C_6H_5OH(p)$	160.84	148.58	155.44	151.68	156.54	154.13	157.66	160.73	170.08	165.83	170.98	167.58	168.22	170.41	171.40	170.69
64 $C_6H_5CHO(o)$	160.95	148.38	155.40	151.51	156.44	154.28	157.59	160.71	170.16	165.91	171.12	167.88	168.58	170.61	171.57	170.79
65 $p-(CH_3O)_2C_6H_4$	161.00	144.87	151.68	147.75	152.47	150.28	153.62	157.63	166.28	162.44	167.44	164.52	164.88	166.94	167.93	167.13
59 $C_6H_5F(p)$	161.00	147.89	154.87	151.31	156.15	153.82	157.32	160.50	169.56	165.52	170.67	167.45	167.98	170.13	171.12	170.37
64 $C_6H_5CHO(m)$	161.92	148.16	154.97	151.14	155.99	153.70	157.20	160.37	169.59	165.38	170.51	167.20	167.88	170.02	171.02	170.23
66 $C_6H_5NO_2(p)$	162.75	147.85	154.60	150.75	155.55	153.26	156.85	160.20	169.69	165.09	170.20	167.04	167.56	169.68	170.79	169.91
59 $C_6H_5F(m)$	163.00	146.66	153.62	149.99	154.80	152.43	155.99	159.19	168.22	164.17	169.29	165.95	166.58	168.74	169.77	168.98
66 $C_6H_5NO_2(m)$	165.12	150.21	157.01	153.16	158.05	155.65	159.30	162.73	171.99	167.68	172.87	169.58	170.15	172.32	173.43	172.57
66 $C_6H_5NO_2(o)$	168.12	155.43	162.80	158.52	163.66	161.46	164.80	168.60	178.64	173.79	179.23	176.32	176.65	178.73	179.71	178.90
67 $C_6H_3F_3$	168.28	154.55	161.06	157.18	162.09	159.82	163.29	168.16	176.98	172.62	177.87	175.32	175.28	177.33	178.41	177.55
68 $C_4H_4N_2$	206.00	187.76	197.09	192.18	198.46	195.31	199.76	201.49	212.87	208.49	215.13	210.16	211.70	214.22	215.73	214.66

[a]See foodnote in Table S4 for label specification.

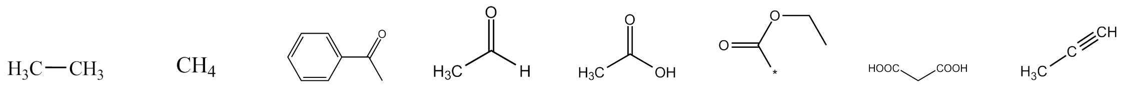
Table S4: Experimental and calculated $^1J_{CH}$ coupling constants[a] that involve *aromatic* carbon (continuation).

Molecule	(16)	(17)	(18)	(19)	(20)	(21)	(22)	(23)	(24)	(25)	(26)	(27)	(28)	(29)	(30)	(31)	(32)	(33)	(34)	(35)
58 $(CH_3)_3C_6H_3$	141.54	149.79	146.51	151.07	148.70	150.84	143.06	148.38	144.48	150.36	146.67	148.75	193.18	188.63	191.46	183.80	190.53	195.91	153.26	150.14
59 $C_6H_5F(o)$	149.78	158.02	154.59	159.31	156.82	159.17	151.29	156.34	152.17	158.16	154.16	156.64	206.00	201.41	203.81	196.73	202.92	207.24	162.06	158.30
60 $C_6H_5NH_2(o)$	141.83	150.60	147.03	151.56	149.06	151.34	143.37	148.63	145.02	150.79	146.95	149.24	193.32	188.88	191.95	184.41	190.66	196.00	153.56	150.57
60 $C_6H_5NH_2(m)$	144.18	152.71	149.25	153.89	151.26	153.65	145.91	151.05	147.19	153.10	149.07	151.50	199.18	194.31	196.74	189.52	195.75	200.40	155.90	152.93
61 $(CH_3)_3C_5H_2N$	145.78	153.68	150.64	155.27	152.66	155.09	147.14	151.94	148.33	154.28	150.29	152.66	197.65	193.05	195.95	188.25	194.78	200.09	157.60	154.18
62 $C_6H_5OH(o)$	144.69	152.99	149.65	154.21	151.74	154.06	146.19	151.18	147.43	153.25	149.37	151.75	197.72	193.21	196.07	188.67	194.91	199.85	156.72	153.22
63 C_6H_6	145.91	154.42	151.03	155.71	153.20	155.53	147.62	152.71	148.94	154.94	150.96	153.34	201.79	197.77	200.32	193.35	198.96	203.44	157.56	154.63
62 $C_6H_5OH(m)$	145.62	154.10	150.63	155.31	152.70	155.11	147.34	152.33	148.51	154.47	150.44	152.90	201.21	196.34	198.72	191.51	197.80	202.31	157.52	154.38
64 $C_6H_5CHO(p)$	146.75	155.36	151.82	156.53	154.04	156.37	148.69	153.71	149.84	155.90	151.91	154.29	204.15	199.88	201.98	195.16	201.07	205.28	158.62	155.52
60 $C_6H_5NH_2(p)$	148.83	157.37	154.02	158.76	156.10	158.53	150.32	155.96	151.74	157.79	153.67	156.17	203.58	199.41	202.49	195.15	200.78	205.71	160.45	157.53
62 $C_6H_5OH(p)$	148.88	157.47	154.00	158.74	156.14	158.54	150.41	155.61	151.72	157.78	153.70	156.17	204.19	199.98	202.94	195.71	201.37	206.08	160.52	157.53
64 $C_6H_5CHO(o)$	148.62	157.30	153.81	158.63	156.14	158.41	150.40	155.74	151.71	157.87	153.91	156.21	205.50	201.25	203.02	196.41	202.67	206.46	160.53	157.56
65 $p-(CH_3O)_2C_6H_4$	145.65	153.57	150.44	155.05	152.57	154.88	146.95	151.77	148.05	153.96	150.05	152.38	198.83	194.18	196.95	189.55	195.82	200.71	157.80	154.16
59 $C_6H_5F(p)$	148.64	157.03	153.71	158.45	155.90	158.27	150.25	155.53	151.46	157.52	153.48	155.93	204.82	200.62	203.38	196.30	201.93	206.40	160.36	157.26
64 $C_6H_5CHO(m)$	148.56	157.13	153.63	158.37	155.85	158.22	150.28	155.34	151.43	157.45	153.46	155.94	205.24	200.63	202.84	195.64	201.96	206.18	160.26	157.26
66 $C_6H_5NO_2(p)$	148.38	156.66	153.34	158.04	155.53	157.98	150.17	155.35	151.20	157.25	153.20	155.70	206.51	202.35	204.58	197.91	203.46	207.45	160.31	156.97
59 $C_6H_5F(m)$	147.43	155.82	152.46	157.19	154.61	157.02	149.16	154.41	150.29	156.31	152.27	154.75	203.83	199.01	201.32	194.12	200.45	204.83	159.55	156.27
66 $C_6H_5NO_2(m)$	150.80	159.35	155.81	160.59	158.01	160.51	152.45	157.47	153.47	159.55	155.46	158.05	208.37	203.46	205.65	198.41	204.89	209.04	162.81	159.58
66 $C_6H_5NO_2(o)$	155.91	164.67	161.10	166.11	163.59	165.90	157.36	162.57	158.43	164.84	160.70	163.06	216.11	212.42	213.74	207.32	213.79	216.78	168.23	164.84
67 $C_6H_3F_3$	155.56	163.61	160.00	164.81	162.28	164.73	156.76	161.47	157.13	163.21	159.11	161.72	212.10	207.44	210.00	203.01	209.18	213.27	168.36	163.73
68 $C_4H_4N_2$	187.57	199.22	194.49	200.63	197.41	200.58	189.33	196.32	191.29	198.86	193.60	197.39	259.99	254.24	256.53	250.02	256.34	257.82	202.74	199.96

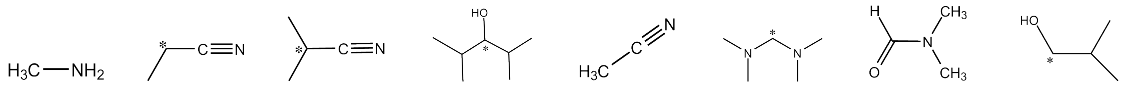
(1) PBE/TZVP, (2) PBE/Huz-IIIsu3, (3) PBE/EPRIII, (4) PBE/aug-cc-pVTZ-J, (5) PBE/ccJ-pVTZ, (6) PBE/pcJ-2, (7) B3LYP/TZVP, (8) B3LYP/Huz-IIIsu3, (9) B3LYP/EPRIII, (10) B3LYP/aug-cc-pVTZ-J, (11) B3LYP/ccJ-pVDZ, (12) B3LYP/ccJ-pVTZ, (13) B3LYP/ccJ-pVQZ, (14) B3LYP/pcJ-2, (15) B3LYP/pcJ-3, (16) B3P86/TZVP, (17) B3P86/Huz-IIIsu3, (18) B3P86/EPRIII, (19) B3P86/aug-cc-pVTZ-J, (20) B3P86/ccJ-pVTZ, (21) B3P86/pcJ-2, (22) B972/TZVP, (23) B972/Huz-IIIsu3, (24) B972/EPRIII, (25) B972/aug-cc-pVTZ-J, (26) B972/ccJ-pVTZ, (27) B972/pcJ-2, (28) M06L/TZVP, (29) M06L/Huz-IIIsu3, (30) M06L/EPRIII, (31) M06L/aug-cc-pVTZ-J, (32) M06L//ccJ-pVTZ, (33) M06L//pcJ-2, (34) B3LYP/TZVP$_g$, (35) B3P86/SAUER$_g$.

Table S5: Molecules[a] studied in this work.

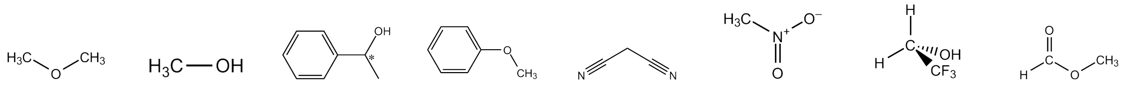
sp^3 hybridized carbon



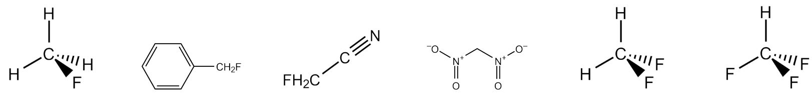
1 2 3 4 5 6 7 8



9 10 11 12 13 14 15 16

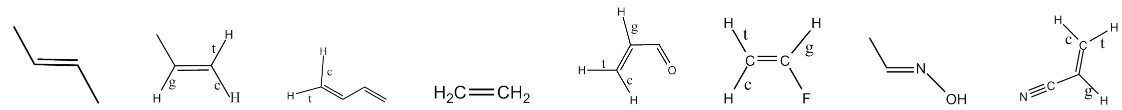


17 18 19 20 21 22 23 24

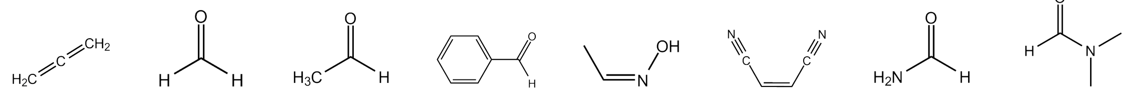


25 26 27 28 29 30

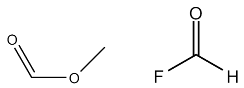
sp^2 hybridized carbon



31 32 33 34 35 36 37 38

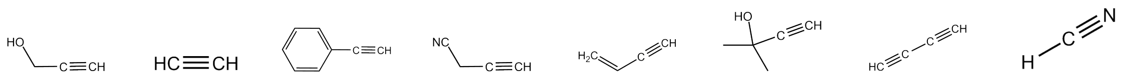


39 40 41 42 43 44 45 46



47 48

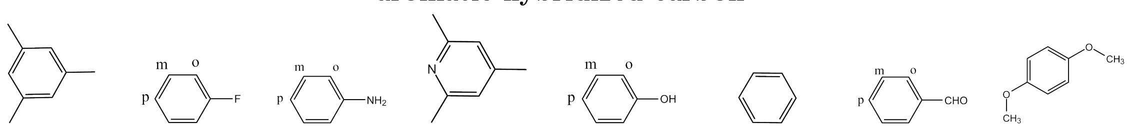
sp hybridized carbon



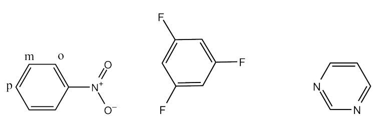
49 50 51 52 53 54 55 56

57

aromatic hybridized carbon



58 59 60 61 62 63 64 65



66 67 68

[a]The molecule number corresponds with that indicated in Tables S1-S4.

Table S6: Statistical results (in Hz) for data set-1 (whole data) using the indicated functional/basis set. Y-intercepts (a), slope (b) and correlation coefficient (r) for fits to Eqs. (2) and (3) of the paper, between parentheses the standard deviation is given.

	Original values					Shifted using Eq.(1)						Scaled using Eq.(1)								5.0 Hz of rovibr. contr.				
Func./Basis set	$\sigma^{(0)}$	mae$^{(0)}$	rmae$^{(0)}$	min$^{(0)}$	max$^{(0)}$	$a^{(1)}$	$\sigma^{(1)}$	mae$^{(1)}$	rmae$^{(1)}$	min$^{(1)}$	max$^{(1)}$	$a^{(2)}$	$b^{(2)}$	r	$\sigma^{(2)}$	mae$^{(2)}$	rmae$^{(2)}$	min$^{(2)}$	max$^{(2)}$	$\sigma^{(r)}$	mae$^{(r)}$	rmae$^{(r)}$	min$^{(r)}$	max$^{(r)}$
PBE/TZVP	16.4	15.6	9.5	-36.3	-4.3	15.61(0.5)	4.7	3.4	1.9	-20.7	11.3	16.79(2.1)	0.99(0.01)	0.993	4.7	3.4	1.9	-21.3	10.4	11.7	10.6	6.4	-31.3	0.7
PBE/HIII-su3	8.5	7.7	4.7	-21.3	8.0	6.94(0.5)	4.8	3.3	1.7	-14.3	14.9	15.43(1.9)	0.95(0.01)	0.994	4.3	3.0	1.7	-18.6	8.9	5.2	3.9	2.1	-16.3	13.0
PBE/EPR-III	12.0	11.1	6.8	-27.7	0.7	11.08(0.5)	4.3	3.1	1.6	-16.6	11.8	14.55(1.9)	0.98(0.01)	0.994	4.3	3.0	1.6	-18.3	9.2	7.5	6.5	3.9	-22.7	5.7
PBE/aug-cc-pVTZ-J	7.6	6.9	4.2	-19.9	10.0	5.89(0.5)	4.8	3.3	1.7	-14.0	15.9	14.92(1.9)	0.95(0.01)	0.994	4.3	3.0	1.6	-18.5	9.2	4.9	3.4	1.8	-14.9	15.0
PBE/ccJ-pVTZ	9.6	8.7	5.3	-25.2	5.4	8.37(0.5)	4.7	3.2	1.7	-16.9	13.8	14.04(2.0)	0.96(0.01)	0.993	4.5	3.1	1.7	-19.7	9.6	5.8	4.6	2.6	-20.2	10.4
PBE/pcJ-2	6.7	6.0	3.6	-19.0	11.0	4.73(0.5)	4.8	3.3	1.7	-14.3	15.7	13.60(1.9)	0.95(0.01)	0.994	4.3	3.0	1.6	-18.7	9.3	4.8	3.3	1.7	-14.0	16.0
B3LYP/TZVP	5.5	4.1	2.3	-16.8	14.6	2.07(0.5)	5.1	3.5	1.9	-14.7	16.7	12.84(2.0)	0.94(0.01)	0.994	4.3	3.1	1.7	-20.0	9.4	5.8	4.2	2.3	-11.8	19.6
B3LYP/HIII-su3	11.2	9.1	5.1	-1.2	30.9	-9.12(0.7)	6.4	4.2	2.3	-10.3	21.8	11.62(1.8)	0.88(0.01)	0.995	4.0	2.8	1.6	-17.4	8.0	15.6	14.1	8.2	3.8	35.9
B3LYP/EPR-III	7.1	5.0	2.7	-5.2	22.8	-4.60(0.6)	5.4	3.6	1.9	-9.8	18.2	10.62(1.8)	0.91(0.01)	0.995	4.0	2.8	1.5	-17.4	8.1	11.1	9.6	5.6	-0.2	27.8
B3LYP/aug-cc-pVTZ-J	12.1	10.1	5.7	-0.0	32.6	-10.14(0.7)	6.5	4.2	2.3	-10.2	22.5	11.16(1.8)	0.88(0.01)	0.995	4.0	2.8	1.5	-17.6	8.1	16.5	15.1	8.8	5.0	37.6
B3LYP/ccJ-pVDZ	9.1	6.9	3.8	-6.1	27.2	-6.59(0.7)	6.2	4.2	2.2	-12.7	20.6	10.57(2.2)	0.90(0.01)	0.993	4.7	3.3	1.8	-20.9	9.1	13.2	11.6	6.8	-1.1	32.2
B3LYP/ccJ-pVTZ	9.5	7.4	4.2	-2.5	27.7	-7.32(0.6)	5.9	3.9	2.1	-9.8	20.4	10.57(1.9)	0.90(0.01)	0.994	4.1	2.9	1.6	-18.4	8.5	13.7	12.3	7.2	2.5	32.7
B3LYP/ccJ-pVQZ	11.5	9.5	5.4	-0.7	31.3	-9.51(0.7)	6.3	4.2	2.2	-10.2	21.8	10.79(1.9)	0.89(0.01)	0.994	4.1	2.9	1.6	-18.0	8.3	15.9	14.5	8.4	4.3	36.3
B3LYP/pcJ-2	12.4	10.6	6.0	0.4	32.9	-10.58(0.7)	6.4	4.2	2.3	-10.1	22.4	10.55(1.8)	0.88(0.01)	0.995	4.0	2.8	1.5	-17.6	8.1	16.9	15.6	9.1	5.4	37.9
B3LYP/pcJ-3	11.8	9.8	5.5	-0.4	31.9	-9.80(0.7)	6.4	4.2	2.3	-10.2	22.1	11.09(1.8)	0.88(0.01)	0.995	4.0	2.8	1.5	-17.5	8.1	16.2	14.8	8.6	4.6	36.9
B3P86/TZVP	15.6	14.9	9.1	-34.3	-4.8	14.94(0.5)	4.3	3.1	1.7	-19.4	10.1	16.03(1.9)	0.99(0.01)	0.994	4.3	3.1	1.7	-20.0	9.8	10.9	9.9	6.0	-29.3	0.2
B3P86/HIII-su3	6.5	5.9	3.5	-16.9	9.8	4.62(0.5)	4.6	3.1	1.7	-12.3	14.4	14.28(1.8)	0.94(0.01)	0.995	3.9	2.7	1.5	-17.3	8.1	4.6	3.1	1.6	-11.9	14.8
B3P86/EPR-III	9.3	8.5	5.2	-23.3	2.8	8.35(0.4)	4.1	2.9	1.5	-15.0	11.2	13.01(1.8)	0.97(0.01)	0.995	3.9	2.7	1.5	-17.3	8.2	5.3	4.3	2.5	-18.3	7.8
B3P86/aug-cc-pVTZ-J	5.7	4.9	2.9	-15.5	12.0	3.25(0.5)	4.6	3.1	1.7	-12.3	15.2	13.48(1.8)	0.94(0.01)	0.995	3.9	2.7	1.5	-17.5	8.1	4.9	3.3	1.7	-10.5	17.0
B3P86/ccJ-pVTZ	7.4	6.7	4.1	-20.3	7.3	5.95(0.5)	4.4	3.0	1.6	-14.4	13.3	13.15(1.8)	0.96(0.01)	0.995	4.0	2.8	1.5	-18.0	8.4	4.5	3.2	1.7	-15.3	12.3
B3P86/pcJ-2	5.8	5.0	2.9	-15.9	11.6	3.46(0.5)	4.6	3.1	1.7	-12.5	15.1	13.44(1.8)	0.94(0.01)	0.995	3.9	2.7	1.5	-17.5	8.1	4.8	3.2	1.7	-10.9	16.6
B97-2/TZVP	14.0	13.2	8.1	-32.7	-2.5	13.15(0.5)	4.5	3.3	1.8	-19.6	10.7	15.75(2.0)	0.98(0.01)	0.993	4.5	3.3	1.8	-20.9	9.5	9.3	8.3	5.0	-27.7	2.5
B97-2/HIII-su3	7.8	6.9	4.2	-21.2	5.3	6.40(0.5)	4.3	3.1	1.7	-14.8	11.7	12.77(1.8)	0.96(0.01)	0.994	4.1	2.9	1.6	-18.0	8.0	4.5	3.4	1.9	-16.2	10.3
B97-2/EPR-III	11.4	10.6	6.5	-28.1	-2.1	10.60(0.4)	4.0	2.9	1.6	-17.5	8.5	11.68(1.9)	0.99(0.01)	0.994	4.1	2.9	1.6	-18.0	7.9	6.9	5.8	3.5	-23.1	2.9
B97-2/aug-cc-pVTZ-J	6.2	5.3	3.2	-18.9	8.8	4.17(0.5)	4.5	3.2	1.7	-14.7	13.0	12.17(1.9)	0.95(0.01)	0.994	4.1	2.9	1.6	-18.7	7.9	4.6	3.2	1.7	-13.9	13.8
B97-2/ccJ-pVTZ	9.5	8.5	5.2	-26.1	1.7	8.45(0.5)	4.3	3.1	1.7	-17.6	10.1	11.72(1.9)	0.98(0.01)	0.994	4.2	3.0	1.6	-19.2	8.3	5.5	4.3	2.5	-21.1	6.7
B97-2/pcJ-2	7.3	6.5	3.9	-20.4	6.9	5.76(0.5)	4.4	3.2	1.7	-14.7	12.7	13.02(1.9)	0.96(0.01)	0.994	4.1	2.9	1.6	-18.3	8.0	4.5	3.3	1.8	-15.4	11.9
M06-L/TZVP	44.8	42.2	24.4	24.5	86.2	-42.17(1.5)	14.5	9.8	5.5	-17.7	44.1	13.55(2.3)	0.74(0.01)	0.991	5.2	3.6	2.0	-27.0	10.5	49.6	47.2	27.5	29.5	91.2
M06-L/HIII-su3	42.8	39.9	23.0	22.8	85.1	-39.89(1.6)	14.9	9.9	5.5	-17.1	45.3	16.43(2.3)	0.73(0.01)	0.991	5.1	3.5	1.9	-27.3	8.8	47.5	44.9	26.1	27.8	90.1
M06-L/EPR-III	43.6	41.2	23.9	24.4	84.2	-41.19(1.5)	13.7	9.4	5.3	-16.8	43.0	11.93(2.3)	0.75(0.01)	0.991	5.1	3.6	2.0	-25.4	9.5	48.4	46.2	27.0	29.4	89.2
M06-L/aug-cc-pVTZ-J	38.2	35.5	20.4	20.1	79.3	-35.48(1.5)	13.7	9.3	5.2	-15.4	43.8	16.25(2.2)	0.75(0.01)	0.992	4.9	3.4	1.9	-25.8	8.5	43.0	40.5	23.5	25.1	84.3
M06-L/ccJ-pVTZ	43.3	40.8	23.7	24.9	83.1	-40.85(1.4)	13.6	9.2	5.2	-16.0	42.3	12.16(2.1)	0.75(0.01)	0.993	4.6	3.2	1.8	-23.6	9.1	48.1	45.8	26.7	29.9	88.1
M06-L/pcJ-2	46.3	44.4	26.0	28.4	83.7	-44.37(1.3)	12.4	8.5	4.8	-15.9	39.3	4.65(2.4)	0.77(0.01)	0.991	5.1	3.7	2.1	-25.9	9.5	51.2	49.4	29.1	33.4	88.7
B3LYP/TZVPg	4.7	3.7	2.1	-12.7	13.4	1.94(0.5)	4.3	2.9	1.6	-10.8	15.3	11.67(1.7)	0.94(0.01)	0.996	3.7	2.6	1.4	-15.7	9.4	5.3	3.8	2.1	-7.7	18.4
B3P86/aug-cc-pVTZ-Jg	5.9	5.3	3.2	-14.7	9.9	4.12(0.4)	4.2	2.9	1.5	-10.6	14.0	13.13(1.6)	0.95(0.01)	0.996	3.6	2.5	1.4	-15.3	7.8	4.3	2.8	1.5	-9.7	14.9

Table S7: Statistical results (in Hz) for data set-2 (sp^3 hybridized carbon atoms) using the indicated functional/basis set. Y-intercepts (a), slope (b) and correlation coefficient (r) for fits to Eqs. (2) and (3) of the paper, between parentheses the standard deviation is given.

	Original values					Shifted using Eq.(1)						Scaled using Eq.(3.)								5.0 Hz of rovibr. contr.				
Func./Basis set	$\sigma^{(0)}$	mae$^{(0)}$	rmae$^{(0)}$	min$^{(0)}$	max$^{(0)}$	$a^{(1)}$	$\sigma^{(1)}$	mae$^{(1)}$	rmae$^{(1)}$	min$^{(1)}$	max$^{(1)}$	$a^{(2)}$	$b^{(2)}$	r	$\sigma^{(2)}$	mae$^{(2)}$	rmae$^{(2)}$	min$^{(2)}$	max$^{(2)}$	$\sigma^{(r)}$	mae$^{(r)}$	rmae$^{(r)}$	min$^{(r)}$	max$^{(r)}$
PBE/TZVP	17.5	16.9	11.7	-25.3	-11.7	16.92(0.6)	3.4	2.5	1.7	-8.3	5.2	0.35(2.7)	1.13(0.02)	0.995	2.3	1.6	1.1	-6.6	3.9	12.6	11.9	8.2	-20.3	-6.7
PBE/HIII-su3	9.5	8.9	6.1	-16.9	-4.2	8.88(0.5)	2.9	2.1	1.5	-8.0	4.7	-1.65(3.0)	1.08(0.02)	0.994	2.4	1.8	1.2	-6.9	4.5	4.9	4.0	2.7	-11.9	0.8
PBE/EPR-III	12.8	12.3	8.4	-20.4	-7.3	12.26(0.6)	3.1	2.3	1.6	-8.2	4.9	-1.30(2.9)	1.10(0.02)	0.995	2.3	1.6	1.1	-6.8	4.3	8.0	7.3	4.9	-15.4	-2.3
PBE/aug-cc-pVTZ-J	8.5	7.9	5.5	-15.6	-3.4	7.95(0.5)	2.7	2.0	1.4	-7.6	4.6	-0.93(2.9)	1.07(0.02)	0.995	2.3	1.6	1.1	-6.7	4.4	4.0	3.2	2.2	-10.6	1.6
PBE/ccJ-pVTZ	10.4	9.8	6.7	-17.7	-4.9	9.79(0.6)	3.0	2.3	1.5	-7.9	4.9	-3.26(2.9)	1.10(0.02)	0.995	2.3	1.7	1.1	-6.6	4.5	5.7	4.8	3.2	-12.7	0.1
PBE/pcJ-2	7.4	6.8	4.6	-14.4	-2.2	6.78(0.5)	2.7	2.0	1.4	-7.6	4.6	-2.42(2.9)	1.07(0.02)	0.995	2.3	1.6	1.1	-6.6	4.4	3.2	2.5	1.7	-9.4	2.8
B3LYP/TZVP	5.6	5.0	3.4	-11.8	-0.9	4.98(0.4)	2.5	1.8	1.2	-6.9	4.1	-5.00(2.5)	1.07(0.02)	0.996	2.0	1.3	0.9	-5.8	3.6	2.5	1.8	1.2	-6.8	4.1
B3LYP/HIII-su3	5.7	5.3	3.8	-1.2	9.2	-5.18(0.4)	2.1	1.5	1.1	-6.4	4.0	-7.02(2.8)	1.01(0.02)	0.995	2.2	1.5	1.1	-6.2	3.9	10.6	10.2	7.2	3.8	14.2
B3LYP/EPR-III	2.7	2.2	1.6	-5.2	5.7	-1.55(0.4)	2.2	1.6	1.1	-6.8	4.2	-7.25(2.7)	1.04(0.02)	0.996	2.1	1.4	1.0	-6.2	4.1	7.0	6.6	4.7	-0.2	10.7
B3LYP/aug-cc-pVTZ-J	6.5	6.1	4.4	-0.0	10.2	-6.11(0.4)	2.0	1.4	1.0	-6.2	4.1	-6.69(2.6)	1.00(0.02)	0.996	2.1	1.4	1.0	-6.1	4.1	11.5	11.1	7.9	5.0	15.2
B3LYP/ccJ-pVDZ	4.2	3.6	2.6	-3.7	7.6	-3.20(0.5)	2.6	2.0	1.4	-6.9	4.4	-14.29(2.8)	1.08(0.02)	0.996	2.1	1.5	1.1	-5.8	4.2	8.7	8.2	5.9	1.3	12.6
B3LYP/ccJ-pVTZ	4.6	4.1	3.0	-2.5	8.2	-3.95(0.4)	2.1	1.5	1.1	-6.4	4.3	-8.23(2.7)	1.03(0.02)	0.996	2.1	1.4	1.0	-6.0	4.2	9.4	9.0	6.4	2.5	13.2
B3LYP/ccJ-pVQZ	6.1	5.7	4.1	-0.7	9.8	-5.65(0.4)	2.1	1.4	1.0	-6.3	4.1	-7.86(2.7)	1.01(0.02)	0.996	2.1	1.4	1.0	-6.1	4.1	11.0	10.7	7.6	4.3	14.8
B3LYP/pcJ-2	7.0	6.6	4.7	0.4	10.7	-6.58(0.4)	2.0	1.4	1.0	-6.1	4.1	-7.40(2.6)	1.01(0.02)	0.996	2.1	1.4	1.0	-6.1	4.1	12.0	11.6	8.2	5.4	15.7
B3LYP/pcJ-3	6.3	5.9	4.2	-0.4	9.9	-5.84(0.4)	2.0	1.4	1.0	-6.2	4.1	-6.95(2.6)	1.01(0.02)	0.996	2.1	1.4	1.0	-6.1	4.0	11.2	10.8	7.7	4.6	14.9
B3P86/TZVP	16.9	16.3	11.3	-24.3	-11.8	16.32(0.6)	3.1	2.2	1.5	-8.0	4.5	0.57(2.4)	1.12(0.02)	0.996	2.0	1.3	0.9	-5.8	4.0	11.9	11.3	7.8	-19.3	-6.8
B3P86/HIII-su3	7.4	6.9	4.7	-14.0	-2.4	6.91(0.4)	2.4	1.8	1.2	-7.1	4.5	-1.61(2.6)	1.06(0.02)	0.996	2.1	1.4	1.0	-6.2	4.3	3.1	2.5	1.7	-9.0	2.6
B3P86/EPR-III	10.4	9.9	6.8	-17.3	-5.2	9.86(0.5)	2.7	2.0	1.4	-7.4	4.6	-2.33(2.6)	1.09(0.02)	0.996	2.1	1.4	1.0	-6.1	4.4	5.7	4.9	3.2	-12.3	-0.2
B3P86/aug-cc-pVTZ-J	6.2	5.6	3.9	-12.5	-1.1	5.64(0.4)	2.3	1.7	1.2	-6.9	4.6	-1.96(2.5)	1.05(0.02)	0.996	2.1	1.4	0.9	-6.1	4.4	2.4	1.7	1.2	-7.5	3.9
B3P86/ccJ-pVTZ	8.3	7.7	5.3	-14.8	-3.1	7.74(0.5)	2.6	1.9	1.3	-7.1	4.6	-2.59(2.6)	1.08(0.02)	0.996	2.1	1.4	1.0	-6.0	4.4	3.8	3.0	2.0	-9.8	1.9
B3P86/pcJ-2	6.4	5.8	4.0	-12.7	-1.3	5.82(0.4)	2.3	1.7	1.2	-6.9	4.6	-1.95(2.5)	1.06(0.02)	0.996	2.0	1.4	0.9	-6.1	4.4	2.5	1.8	1.2	-7.7	3.7
B97-2/TZVP	15.7	15.2	10.5	-22.6	-10.4	15.21(0.5)	3.0	2.1	1.4	-7.4	4.8	1.62(2.5)	1.11(0.02)	0.996	2.1	1.4	1.0	-5.9	3.9	10.8	10.2	7.0	-17.6	-5.4
B97-2/HIII-su3	9.0	8.4	5.8	-15.8	-3.4	8.44(0.5)	2.8	2.1	1.5	-7.3	5.0	-1.66(3.0)	1.07(0.02)	0.994	2.4	1.7	1.2	-6.3	4.2	4.5	3.7	2.5	-10.8	1.6
B97-2/EPR-III	12.3	11.7	8.1	-19.6	-6.6	11.74(0.6)	3.1	2.3	1.6	-7.9	5.2	-2.40(2.9)	1.11(0.02)	0.995	2.3	1.6	1.1	-6.4	4.2	7.5	6.7	4.6	-14.6	-1.6
B97-2/aug-cc-pVTZ-J	7.1	6.5	4.4	-13.8	-1.9	6.50(0.5)	2.6	1.9	1.3	-7.3	4.6	-2.46(2.9)	1.07(0.02)	0.995	2.3	1.6	1.1	-6.3	4.4	3.0	2.3	1.5	-8.8	3.1
B97-2/ccJ-pVTZ	10.5	9.9	6.8	-17.6	-4.7	9.89(0.6)	3.1	2.3	1.5	-7.7	5.2	-3.91(2.9)	1.10(0.02)	0.995	2.4	1.7	1.1	-6.3	4.5	5.9	4.9	3.3	-12.6	0.3
B97-2/pcJ-2	8.5	7.9	5.4	-15.3	-3.2	7.92(0.5)	2.7	2.0	1.4	-7.4	4.7	-1.56(2.9)	1.07(0.02)	0.995	2.3	1.6	1.1	-6.4	4.3	4.0	3.2	2.1	-10.3	1.8
M06-L/TZVP	32.2	30.9	21.3	24.5	60.3	-30.94(1.3)	7.0	4.3	2.7	-6.5	29.4	9.30(2.6)	0.77(0.01)	0.995	2.3	1.5	1.0	-6.7	5.7	37.2	35.9	24.9	29.5	65.3
M06-L/HIII-su3	30.3	29.0	20.0	22.8	56.2	-29.01(1.2)	6.7	4.2	2.7	-6.2	27.2	8.92(2.9)	0.78(0.02)	0.994	2.5	1.8	1.2	-7.0	5.6	35.2	34.0	23.5	27.8	61.2
M06-L/EPR-III	31.6	30.3	20.9	24.4	60.2	-30.31(1.3)	7.1	4.3	2.7	-5.9	29.9	9.55(3.0)	0.77(0.02)	0.993	2.7	1.9	1.3	-7.8	5.8	36.6	35.3	24.4	29.4	65.2
M06-L/aug-cc-pVTZ-J	26.9	25.6	17.6	20.1	52.9	-25.63(1.2)	6.6	4.1	2.6	-5.6	27.2	11.15(2.9)	0.78(0.02)	0.994	2.6	1.9	1.3	-6.8	4.8	31.9	30.6	21.2	25.1	57.9
M06-L/ccJ-pVTZ	31.9	30.5	21.0	24.9	61.5	-30.50(1.3)	7.3	4.4	2.8	-5.7	31.0	10.95(2.7)	0.76(0.02)	0.994	2.4	1.6	1.1	-7.1	5.5	36.8	35.5	24.5	29.9	66.5
M06-L/pcJ-2	35.4	34.3	23.8	28.4	59.0	-34.26(1.1)	6.0	3.7	2.3	-5.8	24.7	0.81(3.1)	0.80(0.02)	0.994	2.5	1.7	1.2	-7.7	6.1	40.4	39.3	27.3	33.4	64.0
B3LYP/TZVPg	4.8	4.3	2.9	-10.8	0.0	4.27(0.4)	2.1	1.5	1.0	-6.5	4.3	0.33(2.5)	1.03(0.02)	0.996	2.1	1.4	1.0	-6.1	4.2	2.3	1.6	1.2	-5.8	5.0
B3P86/aug-cc-pVTZ-Jg	6.6	6.1	4.2	-13.1	-1.4	6.11(0.4)	2.3	1.6	1.1	-7.0	4.7	0.60(2.6)	1.04(0.02)	0.996	2.1	1.4	1.0	-6.4	4.6	2.5	1.9	1.3	-8.1	3.6

Table S8: Statistical results (in Hz) for data set-3 (sp^2 hybridized carbon atoms) using the indicated functional/basis set. Y-intercepts (a), slope (b) and correlation coefficient (r) for fits to Eqs. (2) and (3) of the paper, between parentheses the standard deviation is given.

	Original values					Shifted using Eq.(1)						Scaled using Eq.(1)								5.0 Hz of rovibr. contr.				
Func./Basis set	$\sigma^{(0)}$	mae$^{(0)}$	rmae$^{(0)}$	min$^{(0)}$	max$^{(0)}$	$a^{(1)}$	$\sigma^{(1)}$	mae$^{(1)}$	rmae$^{(1)}$	min$^{(1)}$	max$^{(1)}$	$a^{(2)}$	$b^{(2)}$	r	$\sigma^{(2)}$	mae$^{(2)}$	rmae$^{(2)}$	min$^{(2)}$	max$^{(2)}$	$\sigma^{(r)}$	mae$^{(r)}$	rmae$^{(r)}$	min$^{(r)}$	max$^{(r)}$
PBE/TZVP	18.5	17.4	9.9	-36.3	-12.8	17.38(1.0)	5.4	4.3	2.4	-18.9	4.6	-17.13(4.4)	1.22(0.03)	0.993	3.0	2.1	1.2	-6.3	5.7	13.7	12.4	7.0	-31.3	-7.8
PBE/HIII-su3	9.4	8.3	4.7	-21.3	-4.5	8.31(0.8)	4.0	3.1	1.7	-13.0	3.8	-12.80(4.2)	1.13(0.02)	0.994	2.8	2.2	1.3	-6.4	4.8	5.2	3.4	1.8	-16.3	0.5
PBE/EPR-III	13.4	12.4	7.0	-27.7	-8.4	12.36(0.9)	4.5	3.5	2.0	-15.3	3.9	-13.84(4.2)	1.16(0.03)	0.994	2.9	2.2	1.3	-6.7	4.5	8.8	7.4	4.1	-22.7	-3.4
PBE/aug-cc-pVTZ-J	8.3	7.2	4.0	-19.9	-3.5	7.16(0.8)	4.0	3.1	1.7	-12.7	3.7	-13.65(4.2)	1.13(0.02)	0.994	2.8	2.2	1.2	-6.7	4.6	4.5	2.8	1.5	-14.9	1.5
PBE/ccJ-pVTZ	11.0	9.9	5.5	-25.2	-5.8	9.85(0.9)	4.6	3.6	2.0	-15.4	4.0	-17.60(4.2)	1.17(0.03)	0.994	2.8	2.2	1.3	-6.3	3.8	6.7	4.9	2.6	-20.2	-0.8
PBE/pcJ-2	7.3	6.0	3.3	-19.0	-2.5	5.99(0.8)	4.0	3.2	1.8	-13.0	3.5	-15.85(4.1)	1.13(0.02)	0.994	2.8	2.2	1.2	-6.6	3.5	4.1	2.9	1.6	-14.0	2.5
B3LYP/TZVP	5.3	3.4	1.8	-16.8	0.5	3.34(0.8)	4.1	3.3	1.9	-13.5	3.9	-21.33(4.0)	1.15(0.02)	0.995	2.6	2.1	1.2	-6.0	3.1	4.4	3.8	2.2	-11.8	5.5
B3LYP/HIII-su3	9.0	8.3	5.0	1.1	12.5	-8.34(0.5)	2.8	2.2	1.3	-7.2	4.2	-17.28(3.9)	1.05(0.02)	0.995	2.6	2.1	1.2	-7.0	4.3	13.9	13.3	7.9	6.1	17.5
B3LYP/EPR-III	5.1	4.5	2.7	-5.2	7.9	-3.86(0.6)	3.2	2.5	1.4	-9.1	4.1	-18.37(4.0)	1.08(0.02)	0.995	2.6	2.1	1.2	-6.5	4.3	9.6	8.9	5.3	-0.2	12.9
B3LYP/aug-cc-pVTZ-J	10.0	9.4	5.6	2.8	13.7	-9.45(0.5)	2.8	2.2	1.3	-6.6	4.2	-17.96(3.9)	1.05(0.02)	0.995	2.6	2.1	1.2	-6.4	4.3	15.0	14.4	8.6	7.8	18.7
B3LYP/ccJ-pVDZ	6.9	6.1	3.7	-6.1	9.9	-5.54(0.8)	4.0	3.3	1.9	-11.7	4.4	-28.01(4.6)	1.13(0.03)	0.994	2.9	2.3	1.3	-6.1	3.5	11.5	10.6	6.4	-1.1	14.9
B3LYP/ccJ-pVTZ	7.3	6.6	4.0	-2.3	10.5	-6.41(0.6)	3.2	2.5	1.4	-8.7	4.1	-21.12(4.0)	1.08(0.02)	0.995	2.6	2.1	1.2	-6.1	4.3	12.1	11.4	6.8	2.7	15.5
B3LYP/ccJ-pVQZ	9.4	8.7	5.2	1.6	12.9	-8.74(0.6)	3.0	2.3	1.3	-7.1	4.2	-19.76(4.0)	1.06(0.02)	0.995	2.6	2.1	1.2	-6.4	4.4	14.3	13.7	8.2	6.6	17.9
B3LYP/pcJ-2	10.5	9.9	5.9	3.3	14.2	-9.89(0.5)	2.8	2.2	1.3	-6.6	4.3	-19.09(3.9)	1.05(0.02)	0.995	2.6	2.0	1.2	-6.4	4.5	15.4	14.9	8.8	8.3	19.2
B3LYP/pcJ-3	9.7	9.1	5.4	2.4	13.4	-9.10(0.5)	2.8	2.2	1.3	-6.7	4.3	-18.05(3.9)	1.05(0.02)	0.995	2.6	2.1	1.2	-6.5	4.5	14.6	14.1	8.4	7.4	18.4
B3P86/TZVP	17.5	16.4	9.4	-34.3	-12.3	16.44(1.0)	5.0	3.9	2.1	-17.9	4.1	-16.15(3.7)	1.21(0.02)	0.995	2.5	2.0	1.1	-5.7	3.6	12.7	11.4	6.4	-29.3	-7.3
B3P86/HIII-su3	6.7	5.6	3.1	-16.9	-2.3	5.57(0.7)	3.5	2.7	1.5	-11.4	3.3	-13.15(3.6)	1.11(0.02)	0.995	2.5	2.0	1.1	-6.2	3.5	3.6	2.6	1.4	-11.9	2.7
B3P86/EPR-III	10.3	9.3	5.2	-23.3	-5.9	9.29(0.8)	4.0	3.1	1.7	-14.1	3.4	-14.74(3.7)	1.15(0.02)	0.995	2.5	2.0	1.1	-5.8	3.5	6.0	4.3	2.3	-18.3	-0.9
B3P86/aug-cc-pVTZ-J	5.5	4.1	2.3	-15.5	-0.9	4.13(0.7)	3.5	2.7	1.5	-11.4	3.3	-14.37(3.6)	1.11(0.02)	0.995	2.5	2.0	1.1	-5.8	3.5	3.6	3.0	1.7	-10.5	4.1
B3P86/ccJ-pVTZ	8.2	7.0	3.9	-20.3	-3.6	7.04(0.8)	3.9	3.1	1.7	-13.3	3.4	-16.30(3.6)	1.14(0.02)	0.996	2.4	1.9	1.1	-5.5	3.5	4.4	2.8	1.5	-15.3	1.4
B3P86/pcJ-2	5.6	4.4	2.4	-15.9	-0.9	4.35(0.7)	3.5	2.7	1.5	-11.6	3.4	-14.55(3.6)	1.11(0.02)	0.996	2.4	1.9	1.1	-5.8	3.7	3.6	2.9	1.7	-10.9	4.1
B97-2/TZVP	15.2	14.0	7.9	-32.7	-9.2	13.99(1.0)	5.3	4.2	2.3	-18.7	4.8	-21.47(4.1)	1.22(0.03)	0.995	2.7	2.1	1.2	-5.2	4.3	10.6	9.0	5.0	-27.7	-4.2
B97-2/HIII-su3	8.2	6.8	3.8	-21.2	-1.8	6.85(0.8)	4.3	3.2	1.8	-14.3	5.0	-18.26(4.2)	1.15(0.02)	0.994	2.8	2.1	1.2	-7.1	5.6	4.7	3.0	1.6	-16.2	3.2
B97-2/EPR-III	12.3	11.1	6.2	-28.1	-6.1	11.06(0.9)	4.8	3.6	2.0	-17.0	5.0	-19.58(4.2)	1.19(0.03)	0.994	2.7	2.1	1.2	-6.9	5.8	7.8	6.1	3.3	-23.1	-1.1
B97-2/aug-cc-pVTZ-J	6.3	4.6	2.5	-18.9	0.3	4.54(0.8)	4.2	3.2	1.8	-14.3	4.9	-20.42(4.1)	1.15(0.02)	0.994	2.7	2.1	1.2	-6.8	5.4	4.2	3.3	1.9	-13.9	5.3
B97-2/ccJ-pVTZ	10.4	9.1	5.0	-26.1	-4.1	9.06(0.9)	4.9	3.7	2.0	-17.0	4.9	-22.62(4.1)	1.19(0.02)	0.995	2.7	2.0	1.2	-6.6	5.7	6.4	4.1	2.1	-21.1	0.9
B97-2/pcJ-2	7.6	6.2	3.4	-20.4	-0.8	6.16(0.8)	4.2	3.2	1.8	-14.3	5.4	-18.66(4.1)	1.15(0.02)	0.994	2.8	2.0	1.2	-6.9	6.0	4.4	2.9	1.6	-15.4	4.2
M06-L/TZVP	42.0	41.0	24.1	32.4	46.8	-41.04(0.7)	3.9	2.9	1.7	-8.7	5.8	-35.92(6.4)	0.98(0.03)	0.989	3.9	3.0	1.7	-8.5	5.9	47.1	46.0	27.0	37.4	51.8
M06-L/HIII-su3	40.3	39.3	23.1	30.6	46.2	-39.35(0.7)	3.8	3.0	1.8	-8.7	6.8	-36.65(6.4)	0.99(0.03)	0.989	3.9	3.1	1.8	-8.6	6.9	45.4	44.3	26.1	35.6	51.2
M06-L/EPR-III	42.3	41.4	24.3	31.5	47.8	-41.36(0.8)	3.9	3.1	1.8	-9.9	6.4	-39.30(6.7)	0.99(0.03)	0.988	4.0	3.1	1.8	-9.8	6.5	47.4	46.4	27.3	36.5	52.8
M06-L/aug-cc-pVTZ-J	36.0	35.2	20.7	25.7	42.3	-35.16(0.7)	3.9	3.1	1.8	-9.4	7.1	-33.00(6.4)	0.99(0.03)	0.988	4.0	3.1	1.8	-9.3	7.1	41.1	40.2	23.6	30.7	47.3
M06-L/ccJ-pVTZ	41.8	40.9	24.0	33.5	47.0	-40.91(0.7)	3.4	2.7	1.5	-7.5	6.1	-33.91(5.5)	0.97(0.03)	0.991	3.4	2.7	1.6	-7.2	6.2	46.9	45.9	26.9	38.5	52.0
M06-L/pcJ-2	45.8	44.9	26.4	36.8	51.0	-44.85(0.7)	3.6	2.9	1.7	-8.0	6.1	-51.59(6.3)	1.03(0.03)	0.990	3.6	2.8	1.6	-8.3	6.0	50.9	49.9	29.4	41.8	56.0
B3LYP/TZVPg	4.6	3.3	1.8	-12.7	-0.2	3.28(0.6)	3.2	2.6	1.4	-9.4	3.1	-13.10(3.4)	1.10(0.02)	0.996	2.4	1.8	1.0	-5.7	2.8	3.7	3.2	1.9	-7.7	4.8
B3P86/aug-cc-pVTZ-Jg	5.9	4.9	2.7	-14.7	-1.4	4.92(0.6)	3.2	2.5	1.4	-9.8	3.5	-10.56(3.5)	1.09(0.02)	0.996	2.4	1.9	1.1	-6.2	3.8	3.2	2.5	1.4	-9.7	3.6

Table S9: Statistical results (in Hz) for data set-4 (*sp* hybridized carbon atoms) using the indicated functional/basis set. Y-intercepts (a), slope (b) and correlation coefficient (r) for fits to Eqs. (2) and (3) of the paper, between parentheses the standard deviation is given.

	Original values					Shifted using Eq.(1)						Scaled using Eq.(1)								5.0 Hz of rovibr. contr.				
Func./Basis set	$\sigma^{(0)}$	mae$^{(0)}$	rmae$^{(0)}$	min$^{(0)}$	max$^{(0)}$	$a^{(1)}$	$\sigma^{(1)}$	mae$^{(1)}$	rmae$^{(1)}$	min$^{(1)}$	max$^{(1)}$	$a^{(2)}$	$b^{(2)}$	r	$\sigma^{(2)}$	mae$^{(2)}$	rmae$^{(2)}$	min$^{(2)}$	max$^{(2)}$	$\sigma^{(r)}$	mae$^{(r)}$	rmae$^{(r)}$	min$^{(r)}$	max$^{(r)}$
PBE/TZVP	12.9	11.1	4.3	-24.8	-4.3	11.05(1.8)	5.6	3.7	1.4	-13.8	6.8	58.54(46.9)	0.81(0.19)	0.830	5.6	3.5	1.4	-13.7	4.4	8.5	6.2	2.4	-19.8	0.7
PBE/HIII-su3	6.1	4.6	1.8	-12.5	8.0	-1.94(1.8)	5.7	3.6	1.4	-14.5	6.0	46.06(51.8)	0.81(0.20)	0.819	5.8	3.5	1.3	-14.3	4.9	9.3	8.4	3.3	-7.5	13.0
PBE/EPR-III	8.1	5.5	2.1	-20.1	0.7	5.33(1.8)	5.8	3.6	1.4	-14.8	6.0	52.62(51.3)	0.81(0.20)	0.814	5.9	3.5	1.4	-14.5	4.8	5.8	3.5	1.3	-15.1	5.7
PBE/aug-cc-pVTZ-J	6.7	5.4	2.1	-11.6	10.0	-3.13(1.9)	5.9	3.6	1.4	-14.7	6.9	51.76(50.9)	0.79(0.20)	0.817	5.8	3.5	1.3	-14.4	4.8	10.4	9.4	3.7	-6.6	15.0
PBE/ccJ-pVTZ	6.1	3.5	1.3	-16.2	5.4	1.01(1.9)	6.0	3.7	1.4	-15.2	6.4	54.52(52.0)	0.79(0.20)	0.807	5.9	3.5	1.4	-14.8	4.9	7.3	6.2	2.4	-11.2	10.4
PBE/pcJ-2	7.3	6.3	2.4	-10.7	11.0	-4.14(1.9)	5.9	3.7	1.4	-14.8	6.9	51.59(51.4)	0.79(0.20)	0.815	5.8	3.5	1.3	-14.5	4.8	11.3	10.3	4.0	-5.7	16.0
B3LYP/TZVP	9.5	8.2	3.2	-0.9	14.6	-8.03(1.3)	4.3	3.0	1.2	-8.9	6.6	30.42(37.1)	0.85(0.14)	0.907	4.2	2.8	1.1	-9.6	3.7	14.4	13.0	5.1	4.1	19.6
B3LYP/HIII-su3	26.6	24.9	9.8	16.1	30.9	-24.91(1.3)	4.1	2.7	1.0	-8.9	6.0	12.00(38.4)	0.87(0.14)	0.913	4.1	2.6	1.0	-9.5	3.9	31.8	29.9	11.7	21.1	35.9
B3LYP/EPR-III	18.5	17.0	6.7	7.4	22.8	-17.05(1.3)	4.3	2.8	1.1	-9.7	5.7	16.49(40.5)	0.88(0.15)	0.902	4.3	2.8	1.1	-10.1	4.2	23.6	22.0	8.6	12.4	27.8
B3LYP/aug-cc-pVTZ-J	27.8	26.1	10.2	16.7	32.6	-26.07(1.4)	4.3	2.8	1.1	-9.4	6.5	16.22(40.0)	0.85(0.14)	0.904	4.3	2.7	1.1	-10.0	4.2	33.0	31.1	12.2	21.7	37.6
B3LYP/ccJ-pVDZ	22.7	21.1	8.3	11.6	27.2	-21.10(1.4)	4.3	2.8	1.1	-9.5	6.1	16.44(40.0)	0.86(0.14)	0.904	4.3	2.8	1.1	-10.0	4.3	27.8	26.1	10.2	16.6	32.2
B3LYP/ccJ-pVTZ	23.1	21.6	8.5	11.8	27.7	-21.56(1.4)	4.4	2.8	1.1	-9.8	6.2	17.68(40.8)	0.86(0.15)	0.900	4.4	2.8	1.1	-10.3	4.3	28.3	26.6	10.4	16.8	32.7
B3LYP/ccJ-pVQZ	26.7	25.0	9.8	15.7	31.3	-25.01(1.4)	4.3	2.8	1.1	-9.3	6.3	15.29(39.7)	0.86(0.14)	0.906	4.3	2.7	1.1	-9.9	4.2	31.9	30.0	11.8	20.7	36.3
B3LYP/pcJ-2	28.1	26.4	10.3	17.0	32.9	-26.38(1.4)	4.3	2.8	1.1	-9.3	6.6	16.19(39.9)	0.85(0.14)	0.905	4.3	2.8	1.1	-10.0	4.2	33.4	31.4	12.3	22.0	37.9
B3LYP/pcJ-3	27.2	25.5	10.0	16.4	31.9	-25.52(1.3)	4.2	2.8	1.1	-9.1	6.4	15.35(39.2)	0.85(0.14)	0.908	4.2	2.7	1.0	-9.7	4.2	32.4	30.5	12.0	21.4	36.9
B3P86/TZVP	12.1	10.6	4.1	-21.6	-4.8	10.60(1.5)	4.7	3.1	1.2	-11.0	5.8	42.46(40.6)	0.87(0.17)	0.880	4.8	3.1	1.2	-11.3	4.0	7.5	5.6	2.2	-16.6	0.2
B3P86/HIII-su3	6.7	5.9	2.3	-6.4	9.8	-4.63(1.4)	4.6	2.9	1.1	-11.0	5.2	25.81(42.9)	0.88(0.16)	0.884	4.7	2.9	1.1	-11.3	4.3	11.1	9.9	3.9	-1.4	14.8
B3P86/EPR-III	5.3	3.3	1.3	-13.9	2.8	2.11(1.5)	4.8	3.1	1.2	-11.8	4.9	30.51(44.8)	0.89(0.18)	0.871	4.9	3.1	1.2	-12.0	4.5	5.7	4.7	1.8	-8.9	7.8
B3P86/aug-cc-pVTZ-J	8.1	7.3	2.9	-5.4	12.0	-6.23(1.5)	4.8	3.1	1.2	-11.6	5.7	30.12(44.4)	0.86(0.17)	0.874	4.9	3.0	1.2	-11.9	4.5	12.8	11.3	4.4	-0.4	17.0
B3P86/ccJ-pVTZ	5.3	4.2	1.6	-10.0	7.3	-1.98(1.5)	4.9	3.1	1.2	-11.9	5.4	31.69(45.1)	0.87(0.18)	0.869	5.0	3.1	1.2	-12.1	4.6	8.8	8.0	3.1	-5.0	12.3
B3P86/pcJ-2	7.8	7.0	2.7	-5.6	11.6	-5.87(1.5)	4.8	3.0	1.2	-11.4	5.8	30.18(43.9)	0.86(0.17)	0.876	4.9	3.0	1.2	-11.7	4.5	12.4	11.0	4.3	-0.6	16.6
B97-2/TZVP	9.9	8.2	3.2	-19.5	-2.5	8.21(1.5)	4.8	3.2	1.2	-11.3	5.7	42.24(41.7)	0.86(0.17)	0.875	4.9	3.1	1.2	-11.6	3.9	5.9	3.8	1.5	-14.5	2.5
B97-2/HIII-su3	4.6	3.3	1.3	-10.9	5.3	-0.67(1.4)	4.6	3.0	1.2	-11.6	4.6	23.48(44.1)	0.91(0.17)	0.881	4.8	2.9	1.1	-11.8	3.5	7.5	6.9	2.7	-5.9	10.3
B97-2/EPR-III	8.6	6.6	2.6	-19.4	-2.1	6.60(1.6)	5.0	3.2	1.2	-12.8	4.5	31.20(48.2)	0.90(0.19)	0.855	5.2	3.2	1.2	-12.9	4.5	5.3	3.0	1.1	-14.4	2.9
B97-2/aug-cc-pVTZ-J	6.4	5.6	2.2	-8.7	8.8	-3.86(1.6)	5.0	3.1	1.2	-12.6	5.0	28.68(47.4)	0.87(0.18)	0.861	5.1	3.1	1.2	-12.7	4.4	10.6	9.6	3.8	-3.7	13.8
B97-2/ccJ-pVTZ	5.9	3.5	1.3	-15.8	1.7	2.86(1.6)	5.1	3.2	1.2	-12.9	4.5	31.26(48.5)	0.89(0.19)	0.853	5.2	3.1	1.2	-13.0	4.5	5.5	4.5	1.7	-10.8	6.7
B97-2/pcJ-2	5.4	4.3	1.6	-10.8	6.9	-1.86(1.6)	5.0	3.2	1.2	-12.6	5.1	31.53(47.4)	0.87(0.18)	0.858	5.2	3.1	1.2	-12.7	4.5	8.8	8.0	3.1	-5.8	11.9
M06-L/TZVP	81.1	76.7	30.1	63.0	86.2	-76.74(2.0)	6.3	4.4	1.7	-13.8	9.5	21.28(56.0)	0.71(0.17)	0.828	5.6	3.2	1.2	-13.7	5.2	86.4	81.7	32.0	68.0	91.2
M06-L/HIII-su3	80.8	76.5	30.0	65.5	85.1	-76.47(1.7)	5.3	3.8	1.4	-10.9	8.7	7.36(47.2)	0.75(0.14)	0.881	4.8	3.0	1.1	-11.6	4.4	86.0	81.5	31.9	70.5	90.1
M06-L/EPR-III	77.7	73.4	28.8	58.5	84.2	-73.40(2.1)	6.6	4.1	1.6	-14.9	10.8	34.22(53.3)	0.67(0.16)	0.827	5.7	3.2	1.2	-14.4	4.2	82.9	78.4	30.7	63.5	89.2
M06-L/aug-cc-pVTZ-J	72.8	68.8	27.0	57.6	79.3	-68.84(1.8)	5.6	3.9	1.5	-11.2	10.4	24.59(43.6)	0.71(0.13)	0.882	4.7	2.9	1.1	-11.9	3.4	78.0	73.8	28.9	62.6	84.3
M06-L/ccJ-pVTZ	77.2	73.0	28.6	59.2	83.1	-73.04(2.0)	6.2	4.1	1.5	-13.8	10.1	27.05(52.3)	0.70(0.16)	0.839	5.5	3.1	1.2	-13.7	5.0	82.5	78.0	30.6	64.2	88.1
M06-L/pcJ-2	77.3	73.1	28.6	56.7	83.7	-73.05(2.2)	7.0	4.4	1.7	-16.3	10.6	40.66(57.7)	0.65(0.18)	0.796	6.1	3.4	1.3	-15.3	5.2	82.6	78.1	30.6	61.7	88.7
B3LYP/TZVPg	8.2	7.1	2.8	-1.8	13.4	-6.72(1.3)	4.2	2.9	1.1	-8.5	6.7	31.86(35.5)	0.85(0.14)	0.912	4.1	2.8	1.1	-9.2	3.6	13.0	11.7	4.6	3.2	18.4
B3P86/aug-cc-pVTZ-Jg	6.4	5.6	2.2	-6.7	9.9	-4.24(1.4)	4.6	2.9	1.1	-10.9	5.7	29.37(41.9)	0.87(0.16)	0.886	4.7	2.9	1.1	-11.2	4.3	10.8	9.6	3.8	-1.7	14.9

Table S10: Statistical results (in Hz) for data set-5 (aromatic carbon atoms) using the indicated functional/basis set. Y-intercepts (a), slope (b) and correlation coefficient (r) for fits to Eqs. (2) and (3) of the paper, between parentheses the standard deviation is given.

	Original values					Shifted using Eq.(1)						Scaled using Eq.(1)								5.0 Hz of rovibr. contr.				
Func./Basis set	$\sigma^{(0)}$	mae$^{(0)}$	rmae$^{(0)}$	min$^{(0)}$	max$^{(0)}$	$a^{(1)}$	$\sigma^{(1)}$	mae$^{(1)}$	rmae$^{(1)}$	min$^{(1)}$	max$^{(1)}$	$a^{(2)}$	$b^{(2)}$	r	$\sigma^{(2)}$	mae$^{(2)}$	rmae$^{(2)}$	min$^{(2)}$	max$^{(2)}$	$\sigma^{(r)}$	mae$^{(r)}$	rmae$^{(r)}$	min$^{(r)}$	max$^{(r)}$
PBE/TZVP	14.1	13.6	8.4	-18.2	-6.1	13.61(0.5)	2.3	1.5	0.9	-4.6	7.5	0.77(7.7)	1.09(0.05)	0.979	2.2	1.4	0.8	-2.9	7.5	9.1	8.6	5.3	-13.2	-1.1
PBE/HIII-su3	7.1	6.7	4.1	-9.4	0.7	6.62(0.5)	2.1	1.5	0.9	-2.8	7.3	1.62(7.5)	1.03(0.05)	0.980	2.2	1.4	0.9	-2.8	7.3	2.7	2.2	1.3	-4.4	5.7
PBE/EPR-III	11.0	10.5	6.4	-13.8	-3.0	10.48(0.5)	2.2	1.5	0.9	-3.3	7.5	1.60(7.6)	1.06(0.05)	0.980	2.2	1.4	0.9	-3.0	7.4	6.0	5.7	3.5	-8.8	2.0
PBE/aug-cc-pVTZ-J	6.1	5.8	3.5	-8.5	1.8	5.60(0.5)	2.1	1.4	0.9	-2.9	7.4	1.90(7.5)	1.02(0.05)	0.980	2.2	1.4	0.9	-3.0	7.4	2.2	1.5	0.9	-3.5	6.8
PBE/ccJ-pVTZ	8.4	7.9	4.9	-10.7	-0.4	7.93(0.5)	2.2	1.5	0.9	-2.8	7.5	1.52(7.7)	1.04(0.05)	0.979	2.2	1.4	0.9	-3.0	7.5	3.7	3.4	2.1	-5.7	4.6
PBE/pcJ-2	5.0	4.7	2.9	-7.4	3.0	4.43(0.5)	2.1	1.4	0.9	-2.9	7.4	1.24(7.5)	1.02(0.05)	0.980	2.2	1.4	0.8	-3.0	7.4	2.2	1.4	0.9	-2.4	8.0
B3LYP/TZVP	2.5	1.8	1.1	-4.5	6.9	1.08(0.5)	2.3	1.5	0.9	-3.4	8.0	-6.20(8.4)	1.05(0.05)	0.978	2.3	1.5	0.9	-2.8	8.0	4.6	3.9	2.4	0.5	11.9
B3LYP/HIII-su3	8.7	8.2	5.1	5.2	15.8	-8.24(0.5)	2.2	1.4	0.9	-3.0	7.6	-7.85(8.3)	1.00(0.05)	0.978	2.3	1.4	0.9	-3.0	7.6	13.7	13.2	8.2	10.2	20.8
B3LYP/EPR-III	4.6	4.0	2.5	1.2	11.7	-4.00(0.5)	2.2	1.4	0.9	-2.8	7.7	-5.22(8.0)	1.01(0.05)	0.979	2.2	1.4	0.9	-2.9	7.7	9.5	9.0	5.6	6.2	16.7
B3LYP/aug-cc-pVTZ-J	9.7	9.2	5.7	6.3	16.8	-9.19(0.5)	2.2	1.4	0.9	-2.9	7.6	-4.78(7.9)	0.97(0.05)	0.979	2.2	1.4	0.9	-2.8	7.6	14.7	14.2	8.8	11.3	21.8
B3LYP/ccJ-pVDZ	6.5	5.9	3.7	2.9	13.9	-5.90(0.5)	2.3	1.5	0.9	-2.9	8.0	-6.14(8.5)	1.00(0.05)	0.977	2.3	1.5	0.9	-3.0	8.0	11.4	10.9	6.7	7.9	18.9
B3LYP/ccJ-pVTZ	7.0	6.5	4.0	3.6	14.2	-6.50(0.5)	2.2	1.4	0.9	-2.9	7.7	-4.61(8.0)	0.99(0.05)	0.979	2.2	1.4	0.9	-2.9	7.7	12.0	11.5	7.1	8.6	19.2
B3LYP/ccJ-pVQZ	9.1	8.6	5.3	5.7	16.3	-8.64(0.5)	2.2	1.4	0.9	-2.9	7.7	-5.45(8.0)	0.98(0.05)	0.979	2.2	1.4	0.9	-2.9	7.7	14.1	13.6	8.4	10.7	21.3
B3LYP/pcJ-2	10.1	9.7	6.0	6.8	17.3	-9.66(0.5)	2.2	1.4	0.9	-2.9	7.7	-4.72(7.9)	0.97(0.05)	0.980	2.2	1.4	0.8	-2.8	7.7	15.2	14.7	9.1	11.8	22.3
B3LYP/pcJ-3	9.3	8.9	5.5	6.0	16.5	-8.88(0.5)	2.2	1.4	0.9	-2.9	7.6	-5.02(8.0)	0.98(0.05)	0.979	2.2	1.4	0.9	-2.8	7.6	14.4	13.9	8.6	11.0	21.5
B3P86/TZVP	13.6	13.1	8.0	-18.4	-5.2	13.08(0.5)	2.4	1.5	0.9	-5.3	7.9	-2.12(8.0)	1.10(0.05)	0.979	2.2	1.4	0.9	-2.7	7.9	8.6	8.1	4.9	-13.4	-0.2
B3P86/HIII-su3	5.1	4.8	2.9	-7.4	3.0	4.51(0.5)	2.1	1.3	0.8	-2.9	7.5	-0.39(7.5)	1.03(0.05)	0.980	2.1	1.3	0.8	-3.1	7.5	2.2	1.4	0.8	-2.4	8.0
B3P86/EPR-III	8.5	8.0	4.9	-11.5	-0.4	7.98(0.5)	2.2	1.4	0.9	-3.5	7.6	-1.53(7.6)	1.06(0.05)	0.980	2.2	1.3	0.8	-2.8	7.6	3.8	3.4	2.1	-6.5	4.6
B3P86/aug-cc-pVTZ-J	3.9	3.6	2.2	-5.9	4.3	3.21(0.5)	2.1	1.4	0.8	-2.7	7.5	-1.16(7.6)	1.03(0.05)	0.980	2.2	1.3	0.8	-2.9	7.5	2.8	2.0	1.2	-0.9	9.3
B3P86/ccJ-pVTZ	6.3	6.0	3.6	-8.6	1.8	5.78(0.5)	2.2	1.4	0.8	-2.8	7.6	-0.80(7.6)	1.04(0.05)	0.980	2.2	1.3	0.8	-2.8	7.6	2.3	1.6	1.0	-3.6	6.8
B3P86/pcJ-2	4.0	3.8	2.3	-6.1	4.2	3.38(0.5)	2.1	1.3	0.8	-2.7	7.5	-0.49(7.5)	1.02(0.05)	0.980	2.1	1.3	0.8	-2.9	7.5	2.7	1.9	1.2	-1.1	9.2
B97-2/TZVP	12.0	11.5	7.0	-16.7	-3.7	11.48(0.5)	2.3	1.4	0.9	-5.2	7.8	-3.67(7.9)	1.10(0.05)	0.979	2.2	1.3	0.8	-3.0	7.8	7.0	6.6	4.0	-11.7	1.3
B97-2/HIII-su3	6.8	6.4	3.9	-9.7	1.3	6.28(0.5)	2.2	1.4	0.9	-3.4	7.6	-2.94(7.8)	1.06(0.05)	0.980	2.2	1.3	0.8	-3.2	7.6	2.6	1.9	1.2	-4.7	6.3
B97-2/EPR-III	10.8	10.3	6.3	-14.7	-2.8	10.28(0.5)	2.2	1.4	0.9	-4.4	7.4	-3.52(7.6)	1.09(0.05)	0.981	2.1	1.3	0.8	-3.1	7.4	5.9	5.5	3.3	-9.7	2.2
B97-2/aug-cc-pVTZ-J	4.8	4.5	2.7	-7.1	3.2	4.19(0.5)	2.1	1.4	0.9	-3.0	7.3	-3.92(7.6)	1.05(0.05)	0.981	2.1	1.3	0.8	-3.1	7.3	2.3	1.5	0.9	-2.1	8.2
B97-2/ccJ-pVTZ	8.7	8.2	5.0	-12.4	-0.8	8.25(0.5)	2.2	1.5	0.9	-4.2	7.4	-4.44(7.7)	1.08(0.05)	0.981	2.1	1.3	0.8	-3.1	7.4	4.0	3.6	2.2	-7.4	4.2
B97-2/pcJ-2	6.3	5.9	3.6	-8.6	1.6	5.77(0.5)	2.1	1.4	0.8	-2.9	7.4	-1.99(7.5)	1.05(0.05)	0.981	2.1	1.3	0.8	-3.1	7.4	2.3	1.5	0.9	-3.6	6.6
M06-L/TZVP	44.5	43.2	26.6	37.3	54.0	-43.22(0.9)	4.0	2.6	1.6	-5.9	10.8	5.68(8.2)	0.76(0.04)	0.975	2.4	1.6	1.0	-3.7	7.7	49.6	48.2	29.7	42.3	59.0
M06-L/HIII-su3	39.9	38.7	23.8	32.9	48.2	-38.71(0.9)	3.9	2.7	1.7	-5.8	9.5	7.15(8.6)	0.77(0.04)	0.972	2.5	1.8	1.1	-3.9	7.7	45.0	43.7	26.9	37.9	53.2
M06-L/EPR-III	42.4	41.2	25.3	35.9	50.5	-41.18(0.8)	3.7	2.6	1.6	-5.2	9.3	2.93(8.4)	0.78(0.04)	0.975	2.4	1.7	1.0	-3.7	7.6	47.5	46.2	28.4	40.9	55.5
M06-L/aug-cc-pVTZ-J	35.1	34.1	20.9	28.4	44.0	-34.06(0.9)	4.0	2.9	1.7	-5.7	10.0	11.53(8.3)	0.77(0.04)	0.973	2.5	1.8	1.1	-3.9	7.7	40.2	39.1	24.0	33.4	49.0
M06-L/ccJ-pVTZ	41.4	40.2	24.7	34.7	50.3	-40.21(0.9)	3.9	2.7	1.6	-5.6	10.1	6.62(8.3)	0.77(0.04)	0.974	2.4	1.6	1.0	-3.8	7.7	46.5	45.2	27.8	39.7	55.3
M06-L/pcJ-2	45.8	44.6	27.4	39.7	52.2	-44.55(0.7)	3.2	2.2	1.4	-4.8	7.7	-7.17(8.6)	0.82(0.04)	0.976	2.4	1.5	0.9	-3.7	7.7	50.9	49.6	30.5	44.7	57.2
B3LYP/TZVPg	2.4	1.7	1.0	-3.4	7.1	1.00(0.5)	2.2	1.3	0.8	-2.5	8.1	-2.83(7.9)	1.02(0.05)	0.979	2.2	1.3	0.8	-2.5	8.1	4.6	4.0	2.5	1.6	12.1
B3P86/aug-cc-pVTZ-Jg	4.8	4.6	2.8	-6.8	3.3	4.24(0.5)	2.1	1.3	0.8	-2.6	7.5	0.64(7.3)	1.02(0.05)	0.981	2.1	1.2	0.8	-2.7	7.5	2.2	1.4	0.9	-1.8	8.3

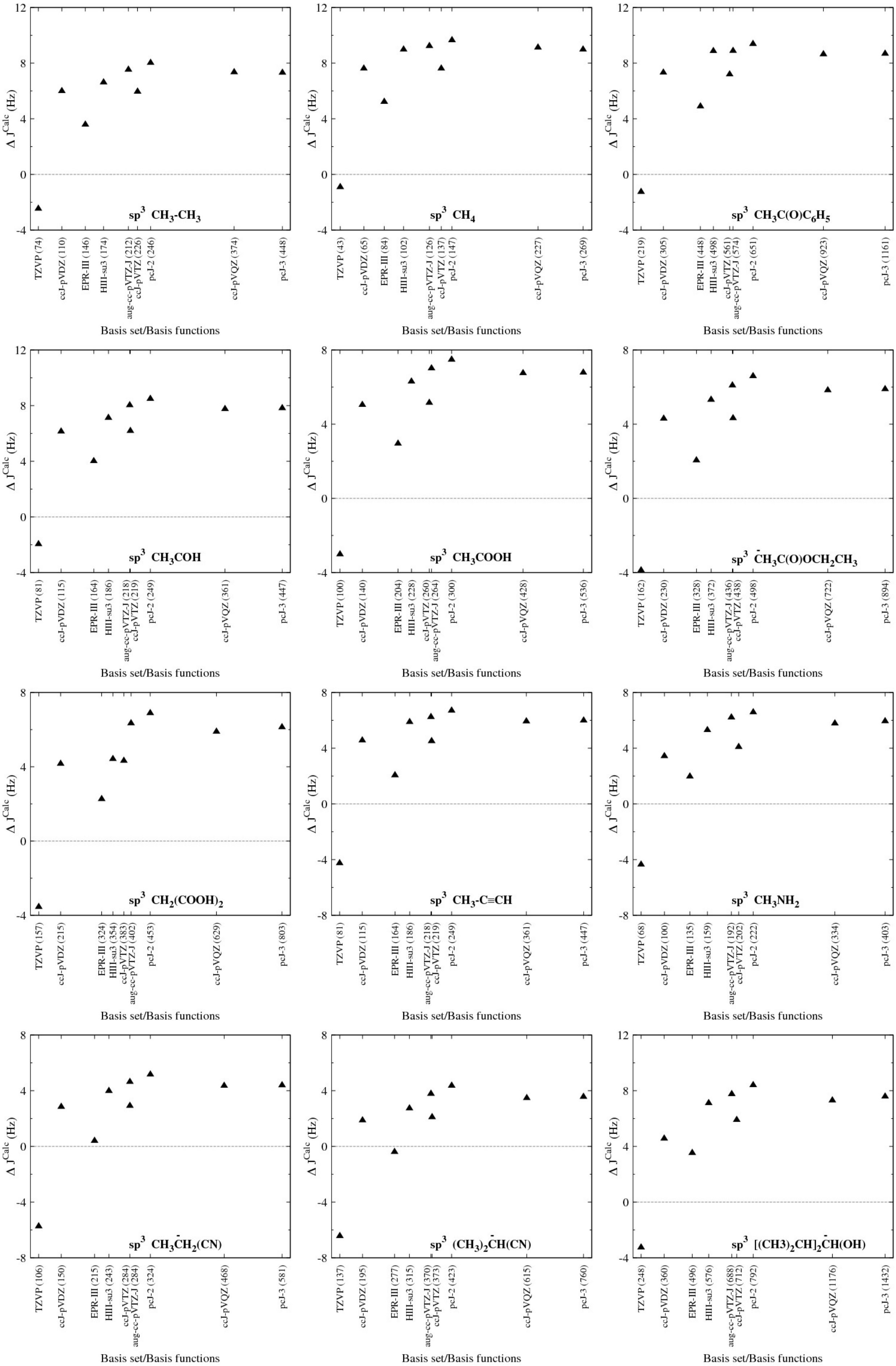


Figure S2: Deviations $\Delta J^{Calc} = \ {}^1J_{CH}^{Calc} - \ {}^1J_{CH}^{Exp}$ against the number of contracted basis functions. B3LYP functional was used.

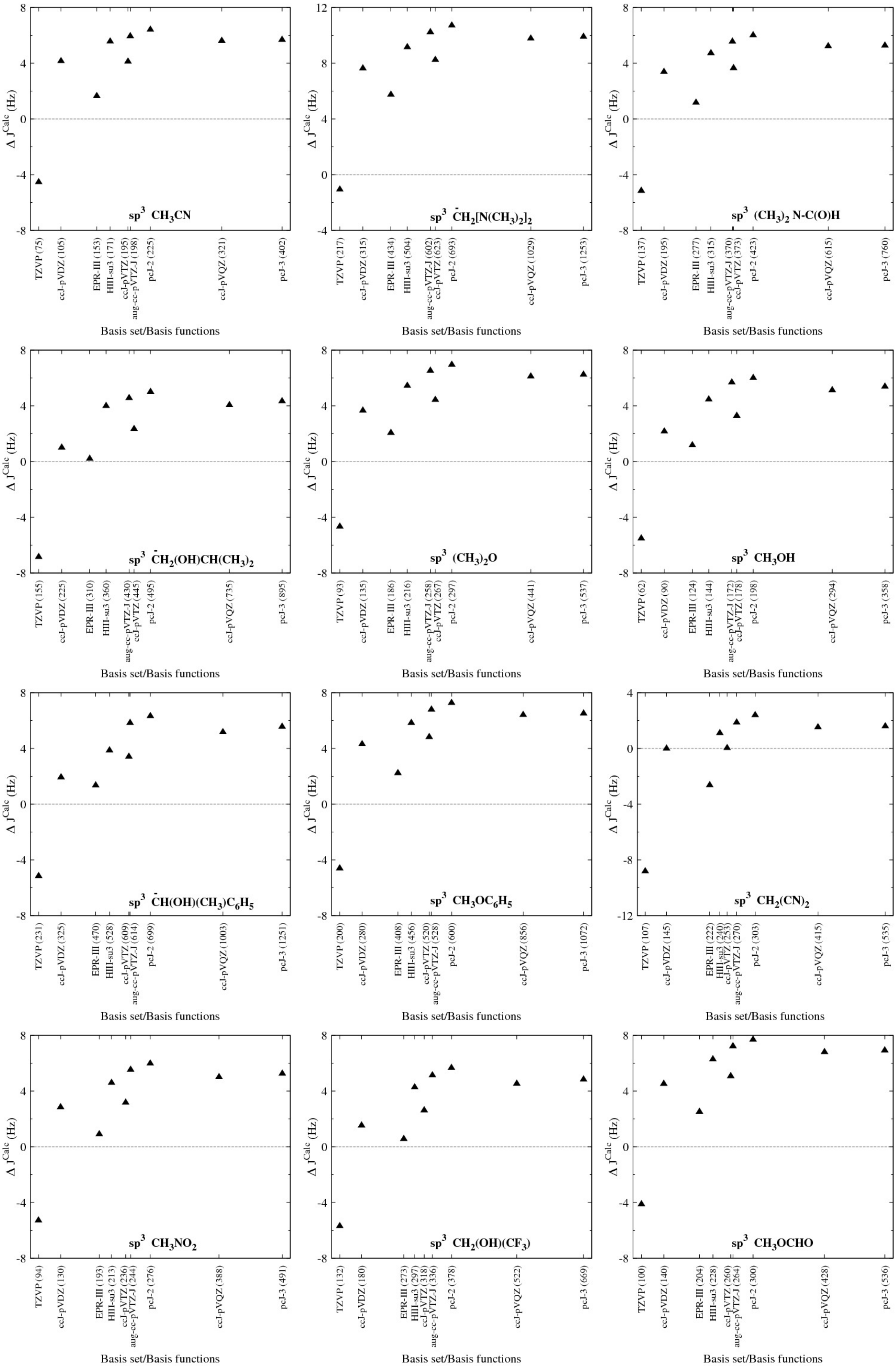


Figure S2: Deviations $\Delta J^{Calc} = \ ^1J_{CH}^{Calc} - \ ^1J_{CH}^{Exp}$ against the number of contracted basis functions. (Continuation, part 2)

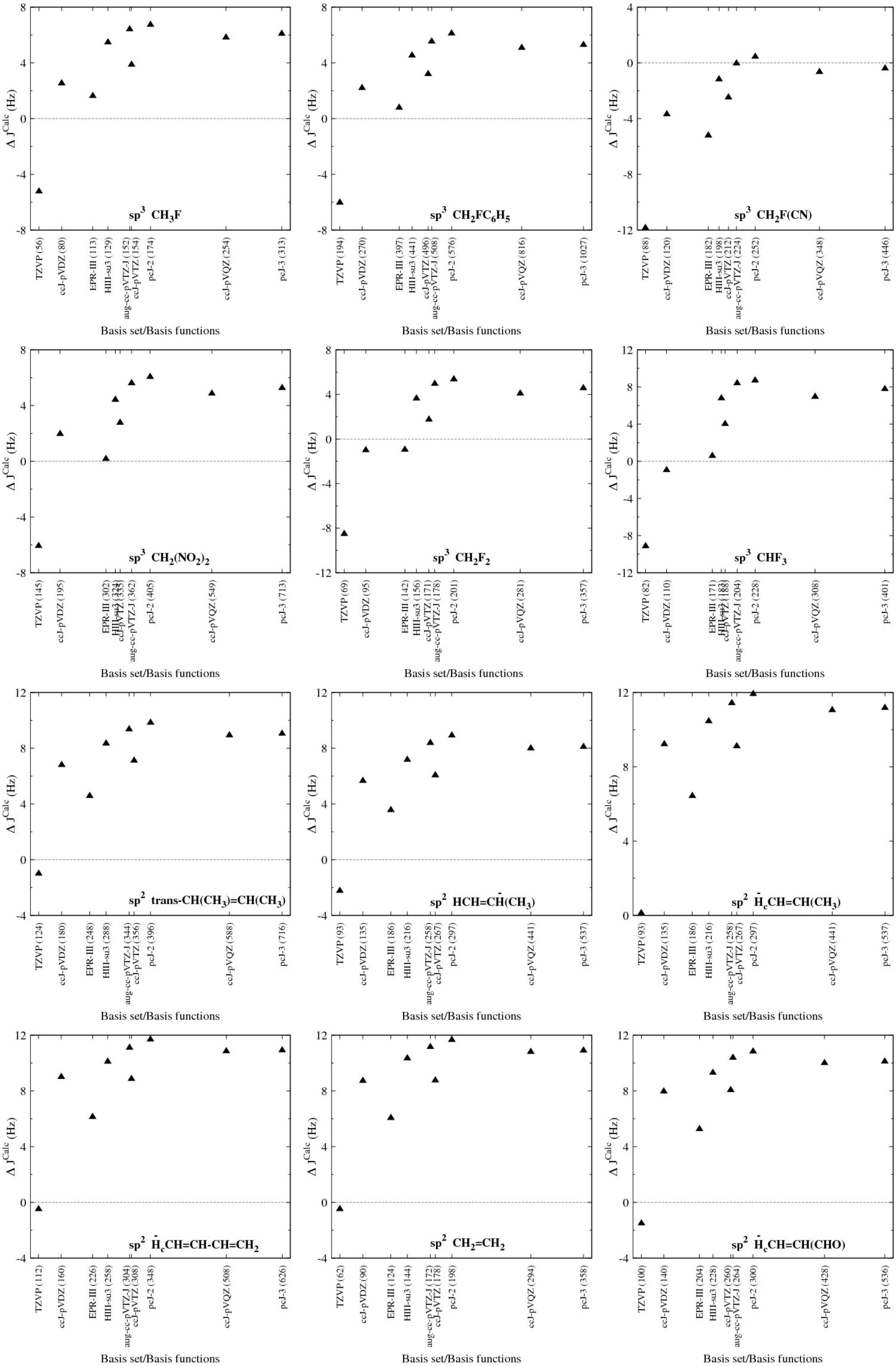


Figure S2: Deviations $\Delta J^{Calc} = \ ^1J_{CH}^{Calc} - \ ^1J_{CH}^{Exp}$ against the number of contracted basis functions. (Continuation, part 3)

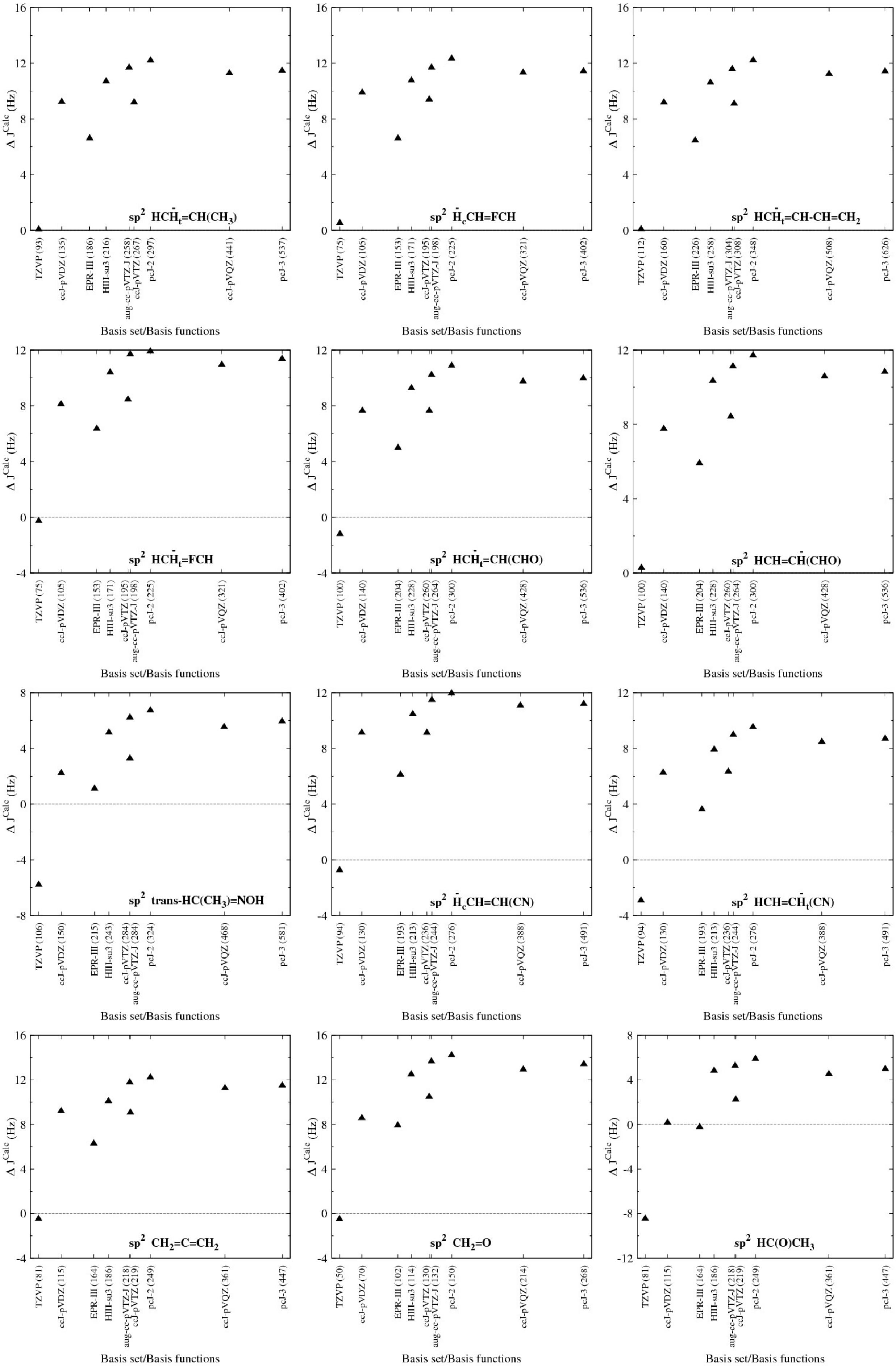


Figure S2: Deviations $\Delta J^{Calc} = \ ^1J^{Calc}_{CH} - \ ^1J^{Exp}_{CH}$ against the number of contracted basis functions. (Continuation, part 4)

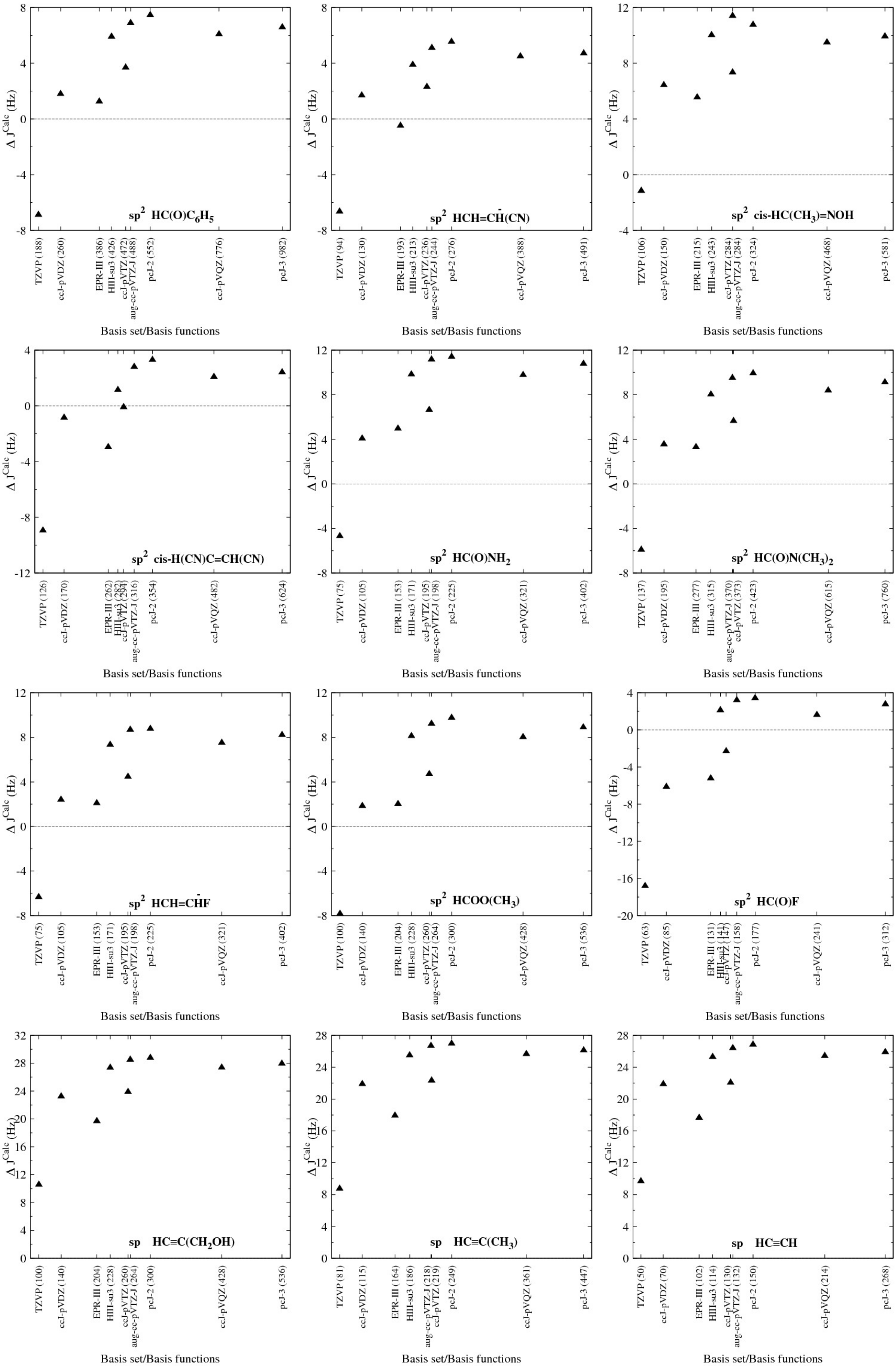


Figure S2: Deviations $\Delta J^{Calc} = {}^{1}J_{CH}^{Calc} - {}^{1}J_{CH}^{Exp}$ against the number of contracted basis functions. (Continuation, part 5)

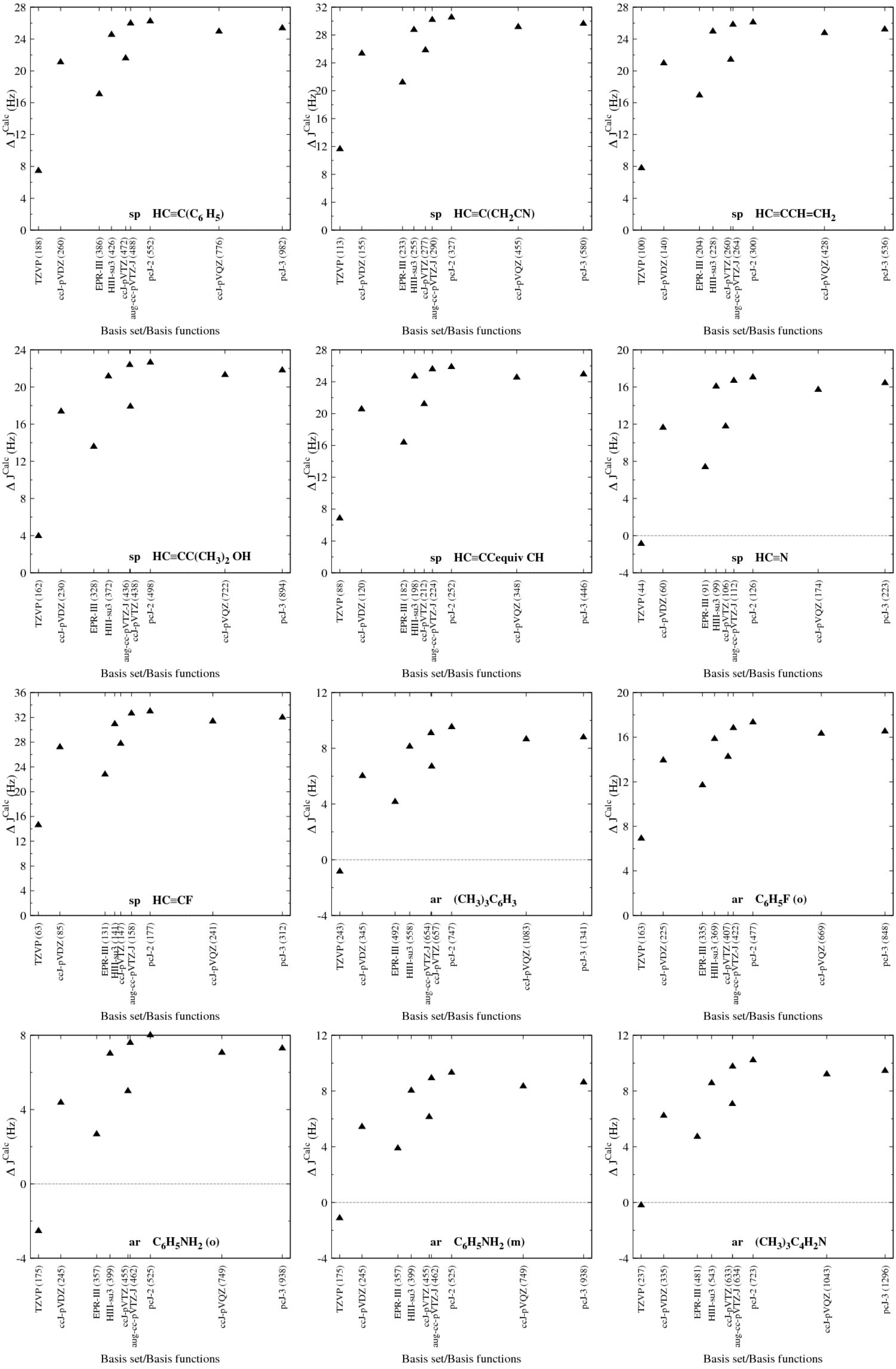


Figure S2: Deviations $\Delta J^{Calc} = {}^{1}J_{CH}^{Calc} - {}^{1}J_{CH}^{Exp}$ against the number of contracted basis functions. (Continuation, part 6)

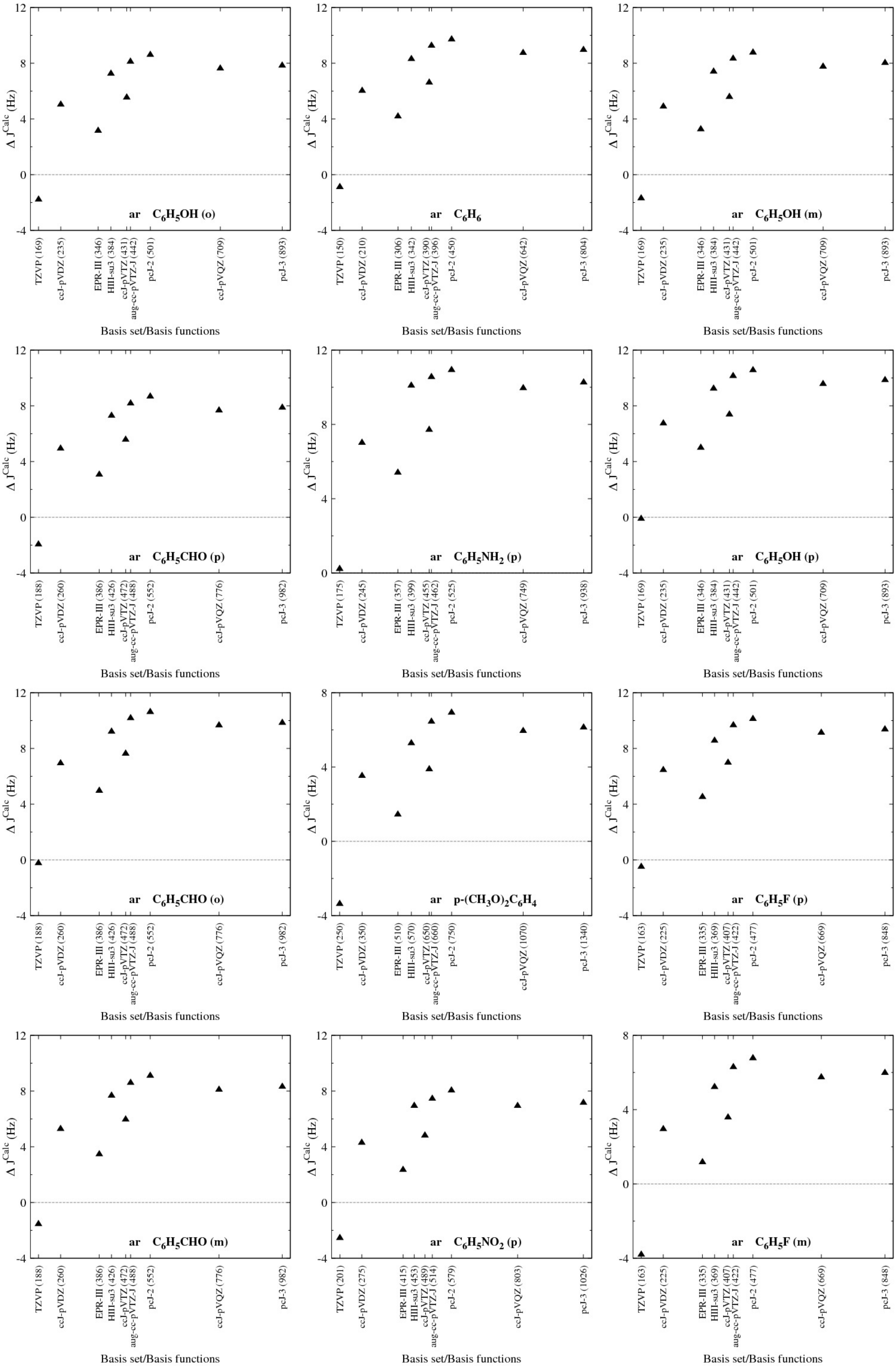


Figure S2: Deviations $\Delta J^{Calc} = {}^1J_{CH}^{Calc} - {}^1J_{CH}^{Exp}$ against the number of contracted basis functions. (Continuation, part 7)

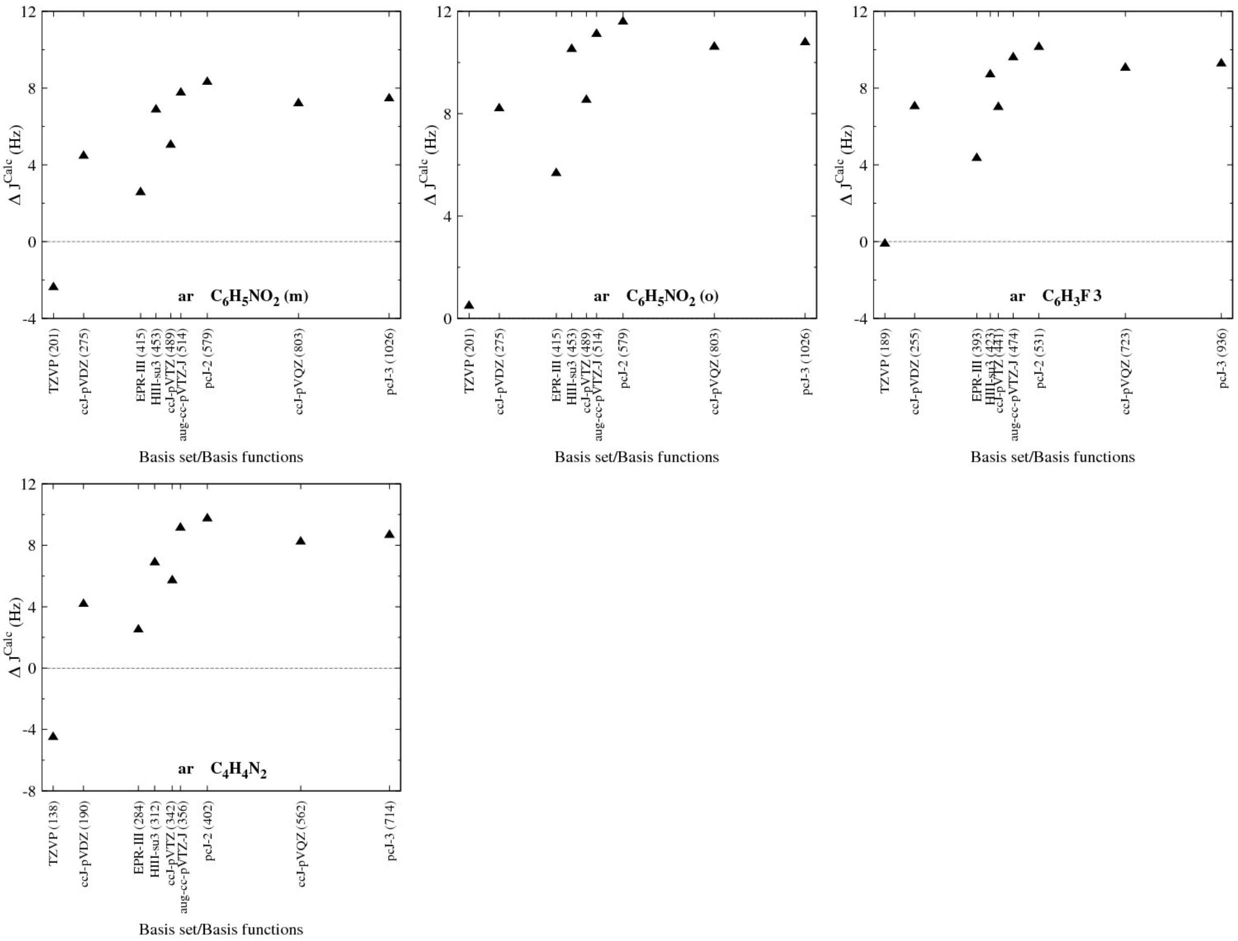


Figure S2: Deviations $\Delta J^{Calc} = {}^1J^{Calc}_{CH} - {}^1J^{Exp}_{CH}$ against the number of contracted basis functions. (Continuation, part 8)

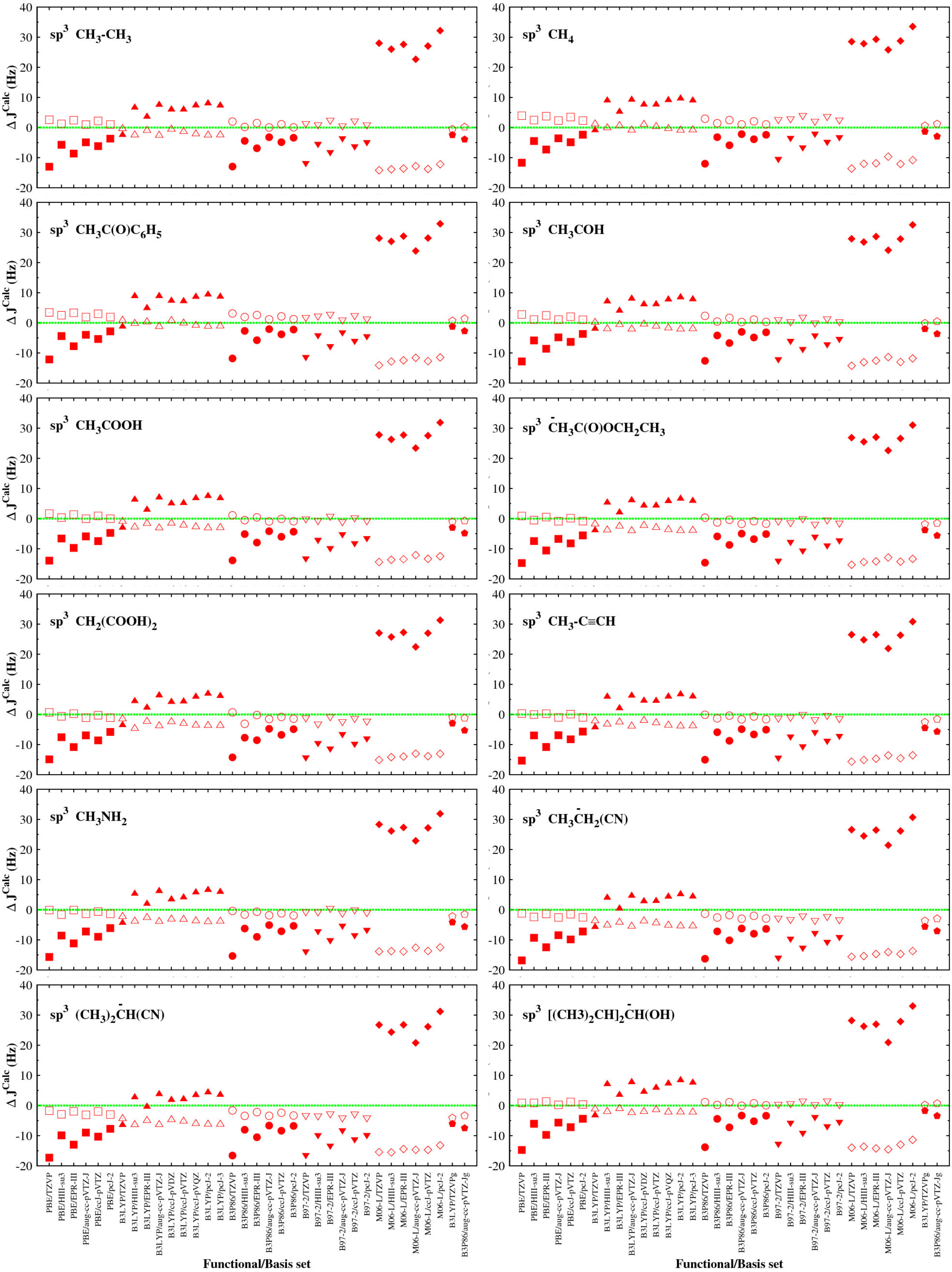


Figure S3: Deviation $\Delta J^{Calc} = {}^1J_{CH}^{Calc} - {}^1J_{CH}^{Exp}$ against the indicated functional/basis set approach. Open symbols correspond to values corrected using the $a^{(1)}$ independent term obtained for the whole set-1.

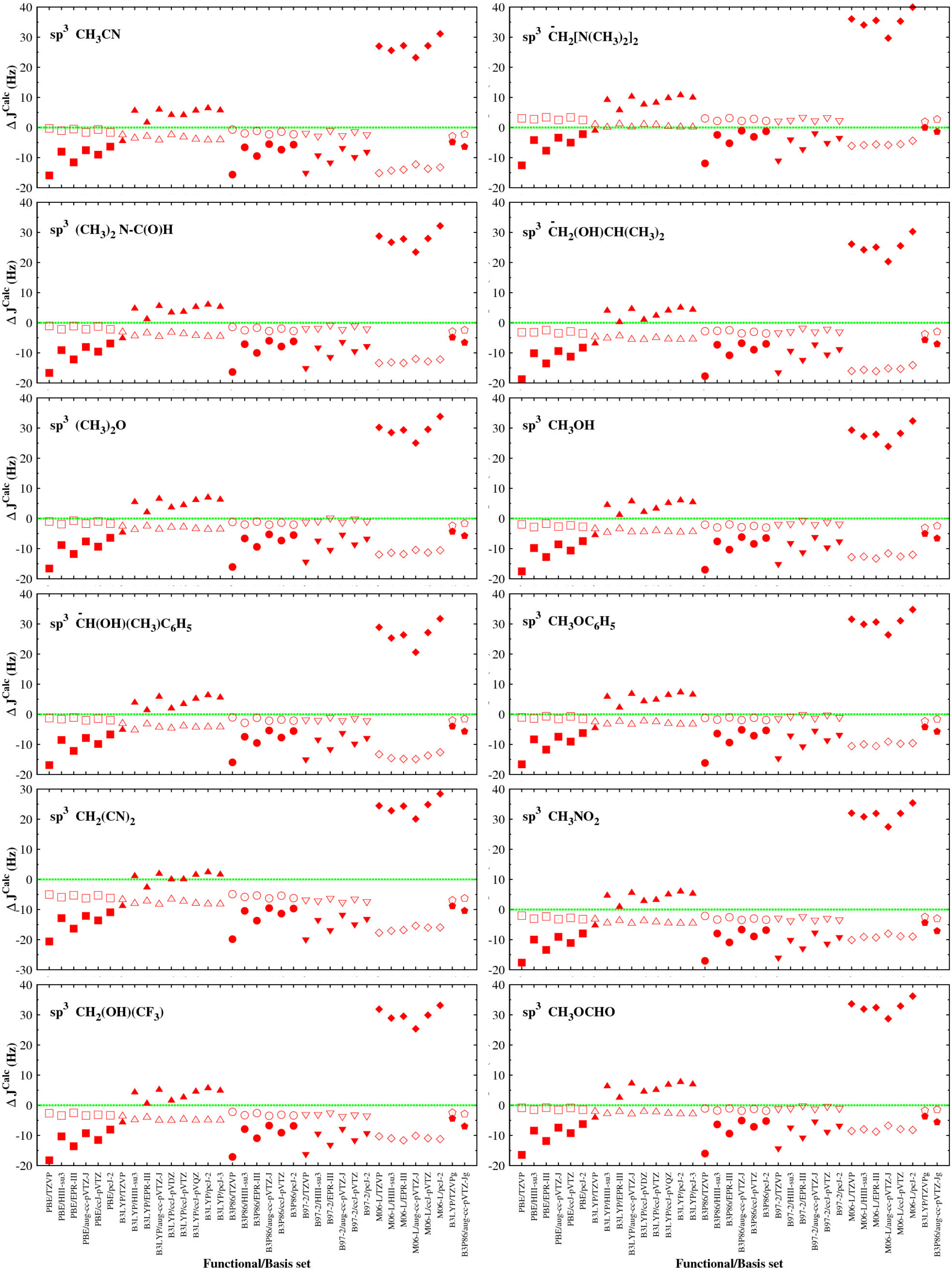


Figure S3: Deviation $\Delta J^{Calc} = {}^{1}J_{CH}^{Calc} - {}^{1}J_{CH}^{Exp}$ against the indicated functional/basis set approach. (Continuation, part 2)

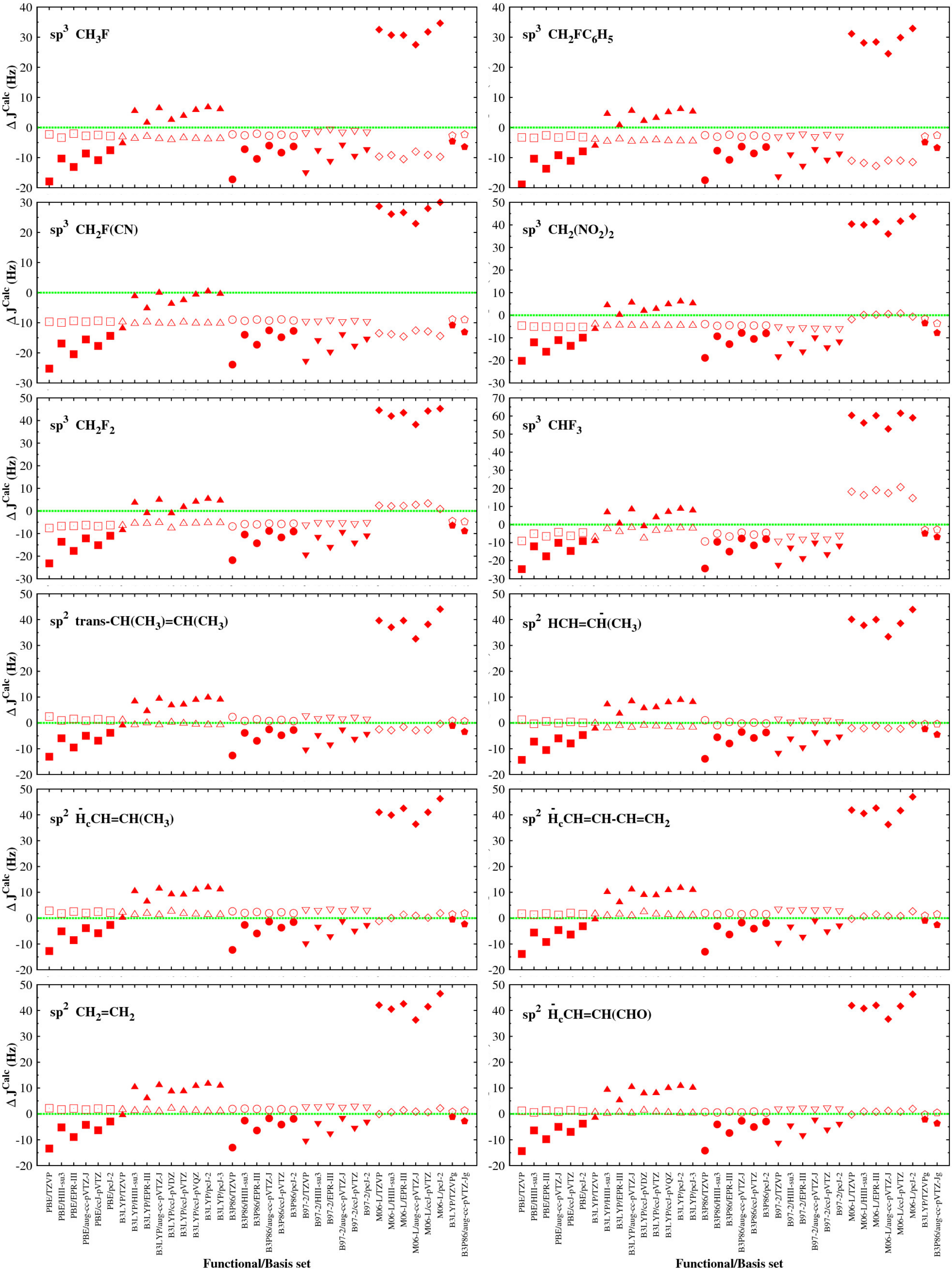


Figure S3: Deviation $\Delta J^{Calc} = {}^1J^{Calc}_{CH} - {}^1J^{Exp}_{CH}$ against the indicated functional/basis set approach. (Continuation, part 3)

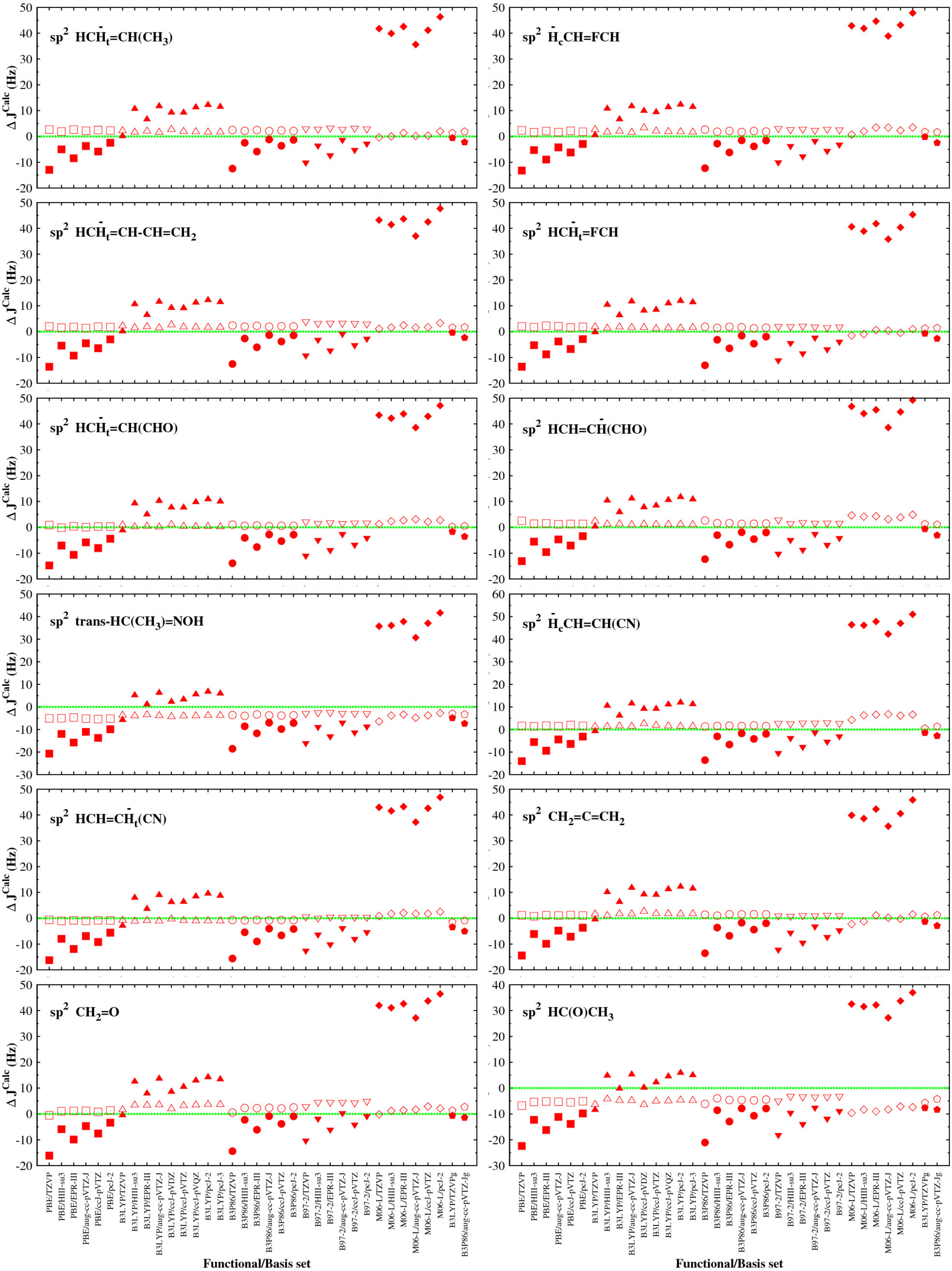


Figure S3: Deviation $\Delta J^{Calc} = ^1J_{CH}^{Calc} - ^1J_{CH}^{Exp}$ against the indicated functional/basis set approach. (Continuation, part 4)

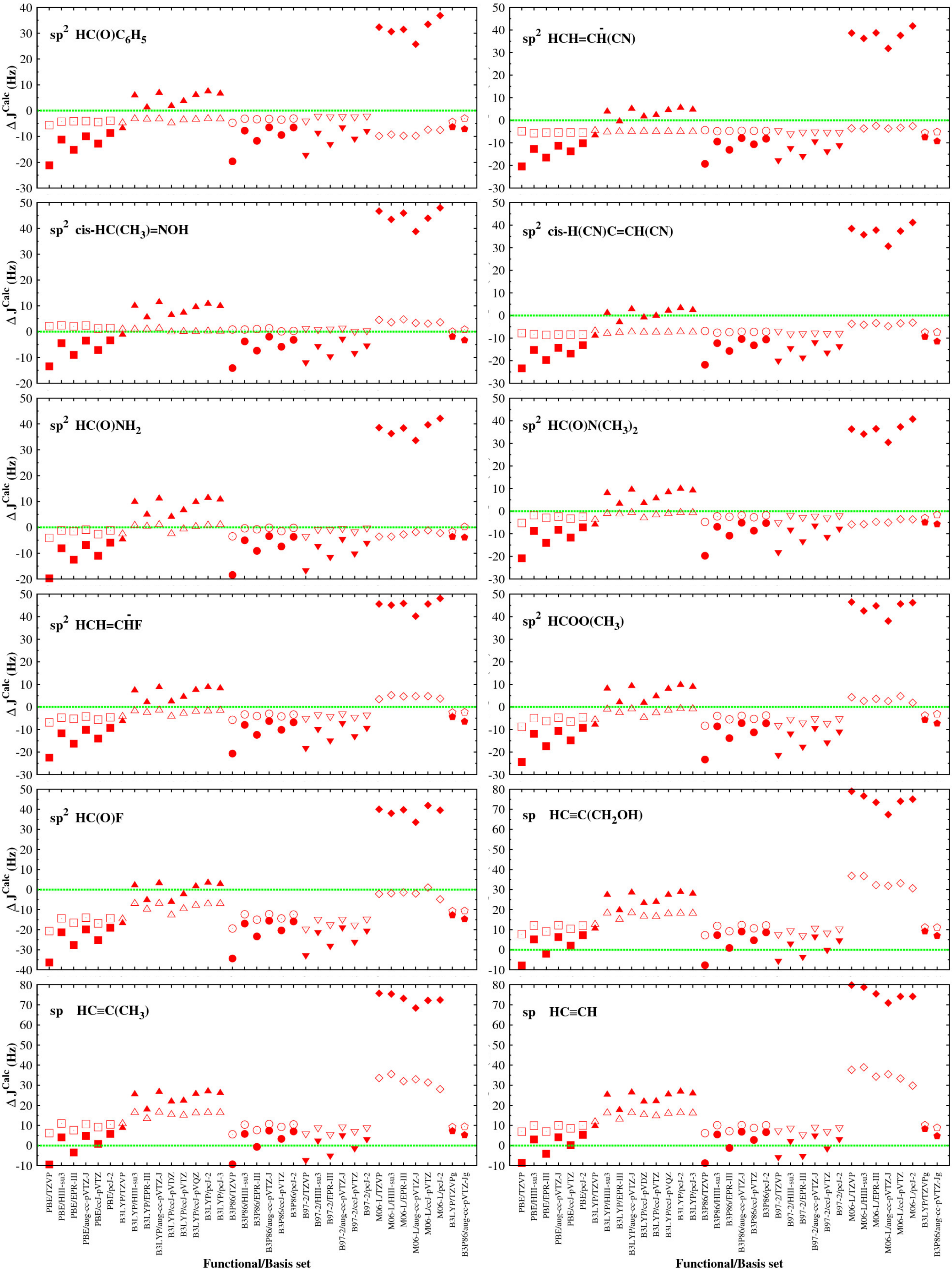


Figure S3: Deviation $\Delta J^{Calc} = {}^{1}J^{Calc}_{CH} - {}^{1}J^{Exp}_{CH}$ against the indicated functional/basis set approach. (Continuation, part 5)

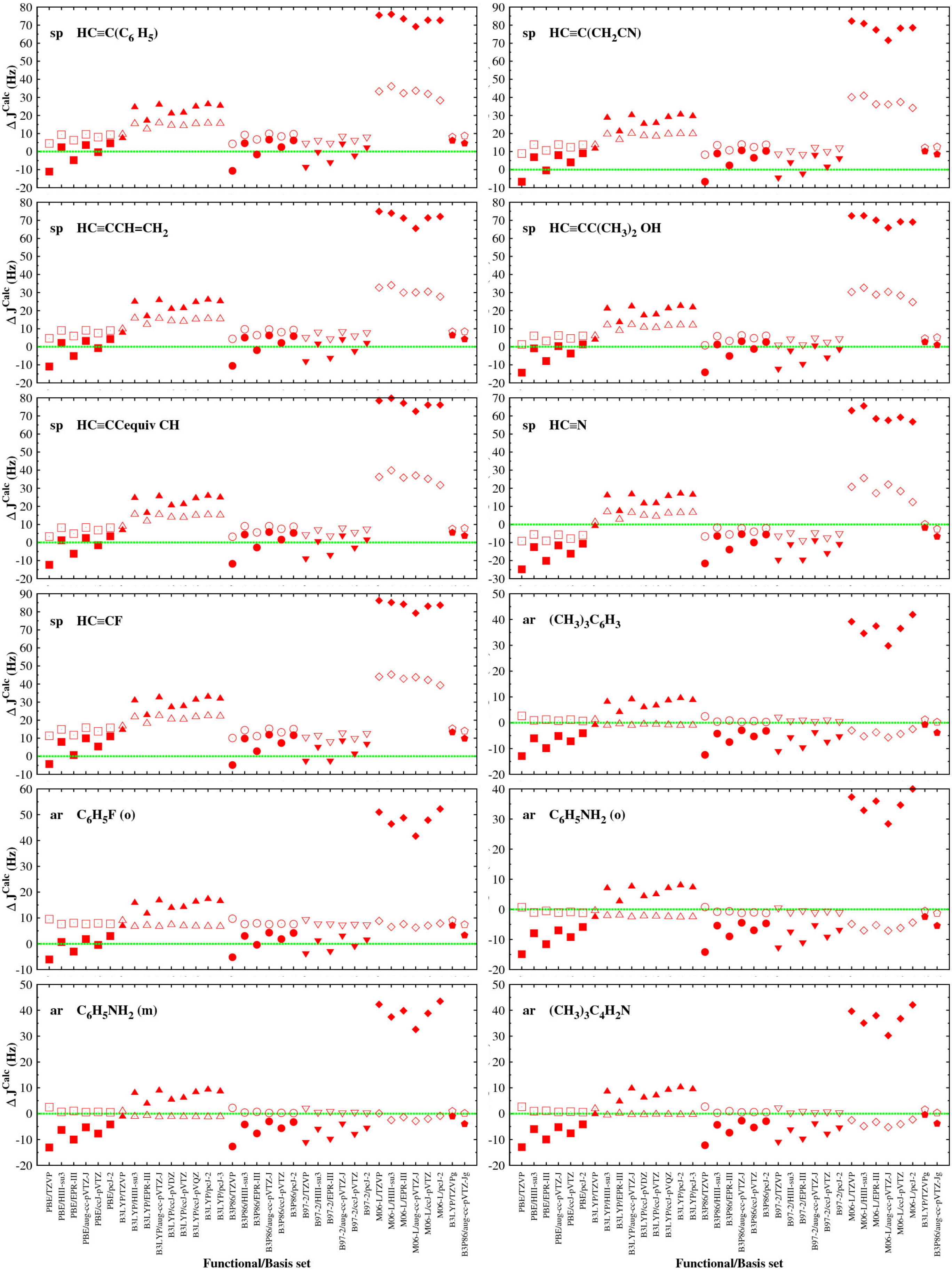


Figure S3: Deviation $\Delta J^{Calc} = {}^1J_{CH}^{Calc} - {}^1J_{CH}^{Exp}$ against the indicated functional/basis set approach. (Continuation, part 6)

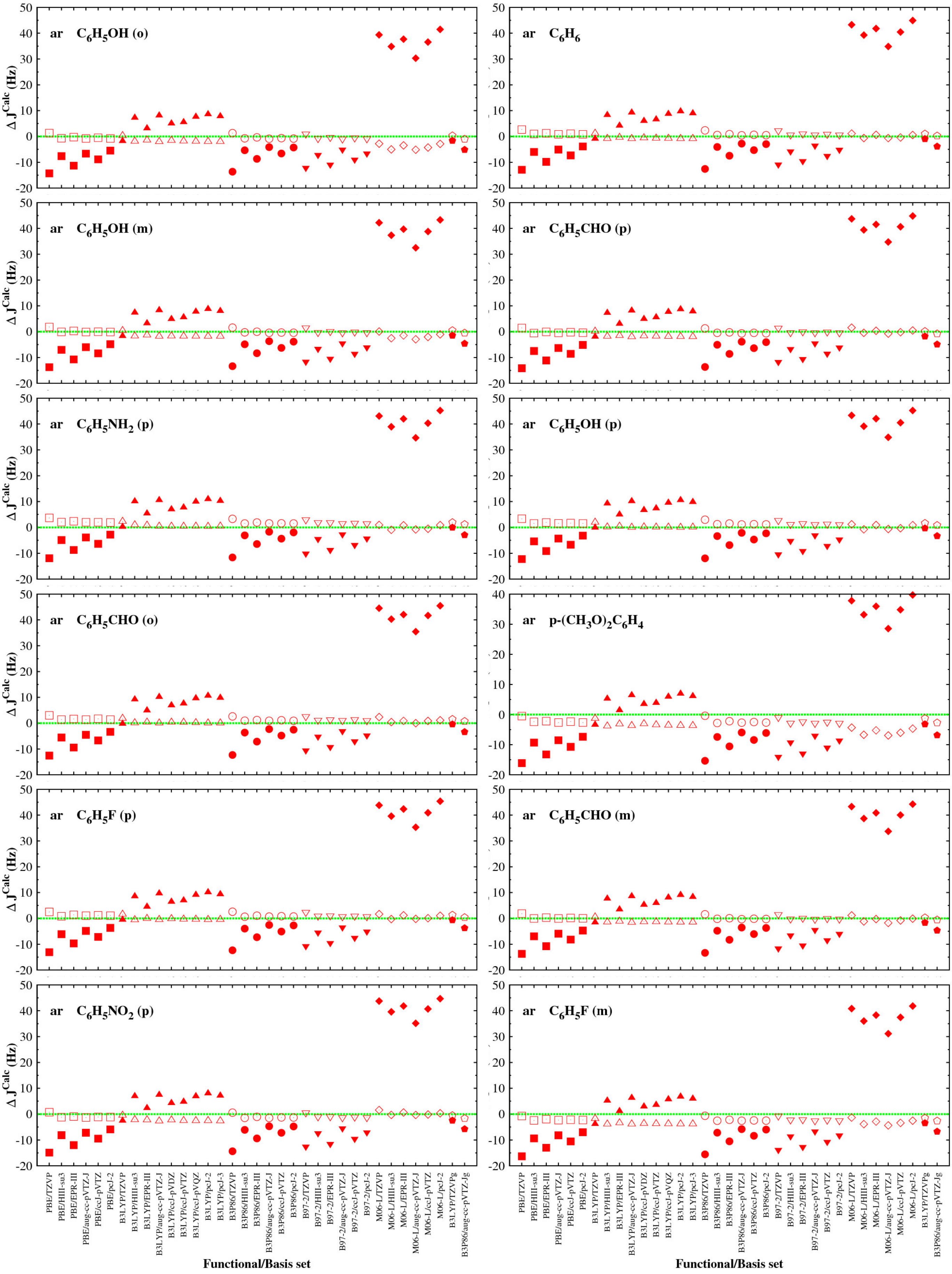


Figure S3: Deviation $\Delta J^{Calc} = {}^1J_{CH}^{Calc} - {}^1J_{CH}^{Exp}$ against the indicated functional/basis set approach. (Continuation, part 7)

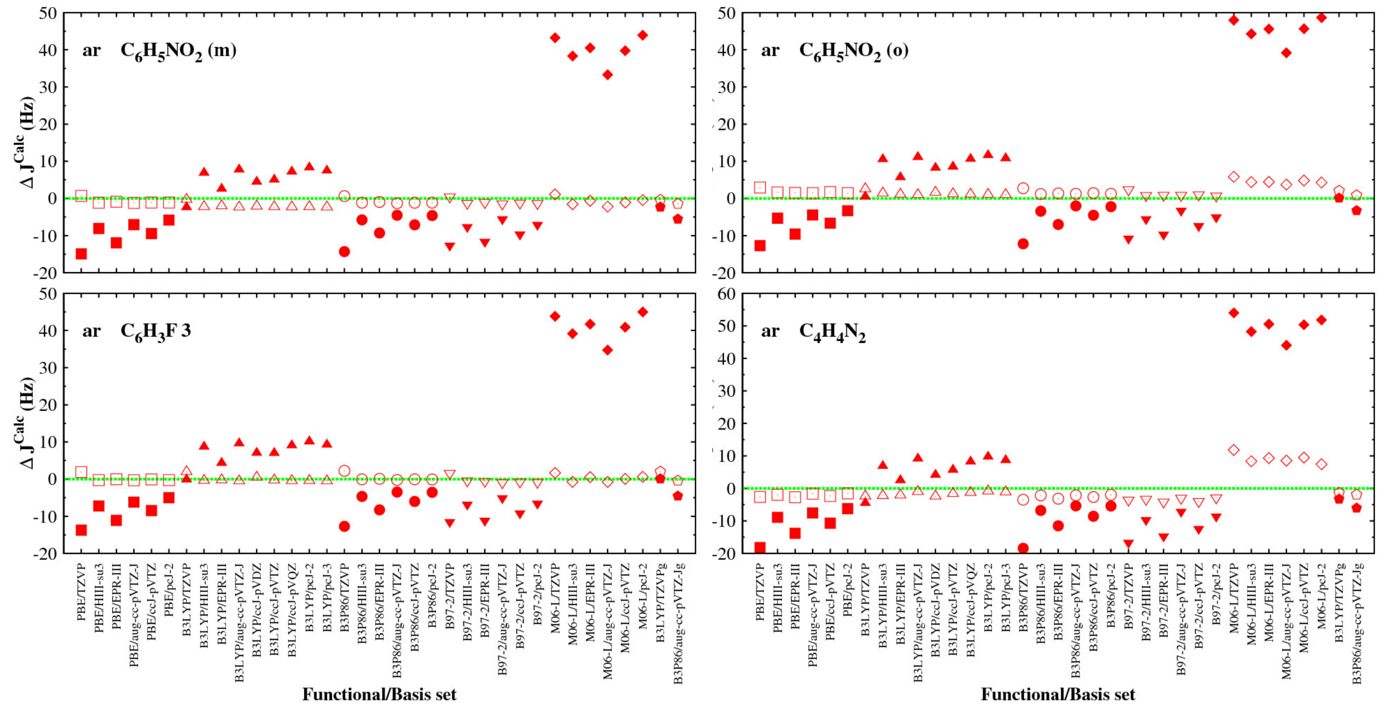


Figure S3: Deviation $\Delta J^{Calc} = {}^1J_{CH}^{Calc} - {}^1J_{CH}^{Exp}$ against the indicated functional/basis set approach. (Continuation, part 8)