Structural and Electronic Effects on One-bond Spin-spin Coupling Constants ^1J(B-N), ^1J(B-H), and ^1J(B-F) for Complexes of Nitrogen Bases with BH_3 and its Fluoro-substituted Derivatives

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Table S1. Components of ^1J(B-N), ^1J(B-H), and ^1J(B-F) (Hz) for Complexes $X:BH_nF_{3-n}$

Complex	PSO	DSO	FC	SD	^1J(B-N)
N2:BH3	0.66	-0.09	7.15	-0.04	7.68
F3N:BH3	0.83	-0.16	8.31	-0.17	8.82
HCN:BH3	0.65	-0.08	-1.24	-0.10	-0.76
H3N:BH3	-0.24	-0.05	-0.12	-0.39	-0.80
H2CNH:BH3	0.50	-0.08	-4.45	-0.22	-4.25
LiCN:BH3	0.53	-0.08	-6.77	-0.18	-6.50
N2:BH2F	0.01	-0.05	-0.86	-0.02	-0.92
F3N:BH2F	0.03	-0.09	-0.78	-0.04	-0.88
HCN:BH2F	0.29	-0.11	6.41	-0.15	6.44
H3N:BH2F	0.17	-0.12	-2.74	-0.33	-3.02
H2CNH:BH2F	0.52	-0.11	-4.34	-0.24	-4.17
LiCN:BH2F	0.28	-0.15	-6.42	-0.22	-6.51
N2:BHF2	0.02	-0.06	0.03	-0.02	-0.03
F3N:BHF2	0.03	-0.09	0.25	-0.03	0.17
HCN:BHF2	0.03	-0.07	0.95	-0.04	0.88
H3N:BHF2	0.17	-0.12	-2.74	-0.33	-3.02
H2CNH:BHF2	0.26	-0.15	-5.88	-0.29	-6.06
LiCN:BHF2	0.28	-0.15	-6.42	-0.22	-6.51
N2:BF3	0.04	-0.08	0.41	-0.02	0.35
F3N:BF3	0.05	-0.11	0.7	-0.03	0.61
HCN:BF3	0.06	-0.1	1.41	-0.04	1.33
H3N:BF3	0.24	-0.16	-12.01	-0.29	-12.23
H2CNH:BF3	0.28	-0.19	-16.16	-0.28	-16.36
LiCN:BF3	0.31	-0.19	-18.91	-0.21	-19.00

$^1J(B-H)$

Complex	PSO	DSO	FC	SD	$^1J(B-H)$
N2:BH3	-0.50	0.50	111.52	0.13	111.65
F3N:BH3	-0.71	0.80	107.86	0.14	108.08
HCN:BH3	-0.38	0.56	101.27	0.10	101.54
H3N:BH3	-0.43	0.53	95.06	0.11	95.26
H2CNH:BH3	-0.42	0.63	94.76	0.11	95.08
LiCN:BH3	-0.32	0.58	93.97	0.08	94.32
N2:BH2F	-1.13	0.69	146.92	0.46	146.94
F3N:BH2F	-1.21	0.82	147.71	0.45	147.77
HCN:BH2F	-0.96	0.97	127.77	0.19	127.97
H3N:BH2F	-0.93	1.01	112.44	0.14	112.66
H2CNH:BH2F	0.08	-0.04	-1.55	-0.05	-1.56
LiCN:BH2F	-0.90	1.03	112.69	0.12	112.94
N2:BHF2	-1.23	1.35	194.38	0.51	195.01
F3N:BHF2	-1.30	1.44	194.77	0.51	195.42
HCN:BHF2	-1.25	1.37	195.62	0.50	196.25
H3N:BHF2	-1.30	1.56	142.80	0.20	143.26
H2CNH:BHF2	-1.36	1.64	142.01	0.19	142.49
LiCN:BHF2	-1.28	1.57	144.90	0.19	145.37

$^1J(B-F)$

Complex	PSO	DSO	FC	SD	$^1J(B-F)$
N2:BH2F	-63.51	0.21	-65.09	-2.00	-130.39
F3N:BH2F	-61.24	0.32	-65.42	-1.90	-128.24
HCN:BH2F	-20.82	0.51	-61.48	1.05	-80.73
H3N:BH2F	-13.39	0.56	-66.60	2.17	-77.27
H2CNH:BH2F	-13.00	0.64	-65.05	2.18	-75.24
LiCN:BH2F	-11.48	0.58	-63.29	2.41	-71.78
N2:BHF2	-47.40	0.74	-37.70	-0.03	-84.38
F3N:BHF2	-47.27	0.83	-38.10	-0.03	-84.57
HCN:BHF2	-45.65	0.77	-34.67	-0.01	-79.56
H3N:BHF2	-21.53	0.98	-44.10	1.50	-63.15
H2CNH:BHF2	-21.81	1.01	-39.86	1.47	-59.19
LiCN:BHF2	-21.70	0.98	-37.57	1.46	-56.83

Complex	PSO	DSO	FC	SD	^{1}J(B-F)
F3N:BF3	-36.75	1.41	45.17	0.36	10.19
HCN:BF3	-35.73	1.35	50.64	0.38	16.64
H3N:BF3	-23.50	1.45	9.97	1.31	-10.76
H2CNH:BF3	-23.68	1.51	14.30	1.28	-6.58
LiCN:BF3	-23.95	1.46	21.31	1.27	0.09

Table S2. MP2/6-311++G(d,p) B-N distances (Å) in complexes X:BH_nF_{3-n}

B-N distances (A)

Acid/Base	NN	NF3	NCH	NH3	NCLi	H2CNH
BH3	1.640	1.642	1.591	1.658	1.576	1.598
BH2F	2.911	2.637	1.724	1.664	1.621	1.623
BHF2	2.974	2.840	2.653	1.675	1.664	1.664
BF3	2.805	2.702	2.446	1.669	1.658	1.662