

Supporting Information

Ab Initio Study of Cooperative Effects in Complexes X:HBO:Z, with X, Z = LiH, HNC, HF, HCN, HCl, ClF, and HBO: Structures, Binding Energies, and Spin-Spin Coupling Constants across Intermolecular Bonds

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Pg. 01 - 14: Table S1. Coordinates of complexes X:HBO:Z

Pg. 15 - 16: Table S2. MP2/aug'-cc-pVTZ binding energies of ternary complexes, binary complexes isolated and in ternary complexes, and enhanced binding energies of ternary complexes X:HBO:Z (kJ/mol) for fixed Z as a function of X

Pg. 17 – 23: Table S3. Spin-spin coupling constants (Hz) for the B-H...A interaction in complexes X:HBO:Z for fixed X as a function of Z, with A the atom of X interacting with B-H

Pg. 24 – 30: Table S4. Spin-spin coupling constants (Hz) for the H-Li...O, D-H...O, and F-Cl...O interactions in complexes X:HBO:Z for fixed Z as a function of X

Table S1. Coordinates of ternary complexes X:HBO:Z

X:HBO:Z	Cartesian Coordinates
LiH:HBO:LiH	O,0.0944355297,0.,0.
MP2= -116.60895084	B,1.313949253,0.,0.
	H,2.491447226,0.,0.
	Li,-1.824418134,0.,0.
	H,-3.4630132032,0.,0.
	H,4.4874114359,0.,0.
	Li,6.0945445127,0.,0.
LiH:HBO:HNC	O,0.0735663708,0.,0.
MP2= -201.80918656	B,1.2924124966,0.,0.
	H,2.467479258,0.,0.
	H,-1.704838814,0.,0.
	N,-2.7205165393,0.,0.
	C,-3.8965889803,0.,0.
	H,4.5520366343,0.,0.
	Li,6.1577453339,0.,0.
LiH:HBO:HF	O,0.0880680548,0.,0.
MP2= -208.91721698	B,1.3056935157,0.,0.
	H,2.4807910325,0.,0.
	H,-1.6378361402,0.,0.
	F,-2.574468372,0.,0.
	H,4.5798663072,0.,0.
	Li,6.185684872,0.,0.
LiH:HBO:HCN	O,0.0700513236,0.,0.
MP2= -201.83162188	B,1.2887226587,0.,0.
	H,2.4631274819,0.,0.
	H,-1.9400649478,0.,0.
	C,-3.0144899041,0.,0.
	N,-4.181926351,0.,0.
	H,4.5874477958,0.,0.
	Li,6.1925361428,0.,0.
LiH:HBO:HCl	O,0.0835070848,0.,0.
MP2= -568.88663279	B,1.3019754491,0.,0.
	H,2.4761465715,0.,0.
	H,-1.7880948335,0.,0.
	Cl,-3.0786817274,0.,0.
	H,4.602223427,0.,0.
	Li,6.2071532385,0.,0.
LiH:HBO:ClF	O,0.0832745414,0.,0.
MP2= -667.93315373	B,1.3015675908,0.,0.
	H,2.4755801354,0.,0.
	Cl,-2.4439853405,0.,0.
	F,-4.0987223992,0.,0.
	H,4.6166828737,0.,0.
	Li,6.2212890884,0.,0.

LiH:HBO:HBO
MP2= -209.10801351

O,0.0664248206,0.,0.
B,1.2849524893,0.,0.
H,2.4586261597,0.,0.
H,-2.299013954,0.,0.
B,-3.4688210056,0.,0.
O,-4.68586653,0.,0.
H,4.6292037863,0.,0.
Li,6.2338949039,0.,0.

HBO:HBO:LiH
MP2= -209.13017029

O
X,1,1.
B,1,r1,2,90.
H,1,r2,2,90.,3,0.,0
Li,1,r3,2,90.,3,180.,0
H,1,r4,2,90.,3,180.,0
O,1,r32,2,90.,3,0.,0
B,1,r42,2,90.,3,0.,0
H,1,r52,2,90.,3,0.,0

r1=1.21736784
r2=2.38648801
r3=1.93107147
r4=3.56414274
r32=4.65476451
r42=5.87097322
r52=7.03783157

HBO:HBO:HNC
MP2= -294.33183714

O
X,1,1.
B,1,r1,2,90.
H,1,r2,2,90.,3,0.,0
H,1,r3,2,90.,3,180.,0
N,1,r4,2,90.,3,180.,0
C,1,r5,2,90.,3,180.,0
O,1,r32,2,90.,3,0.,0
B,1,r42,2,90.,3,0.,0
H,1,r52,2,90.,3,0.,0

r1=1.21698456
r2=2.38589566
r3=1.80177318
r4=2.81520128
r5=3.99140597
r32=4.72003056
r42=5.93595726
r52=7.10278049

HBO:HBO:HF
MP2= -301.44019423

O
X,1,1.
B,1,r1,2,90.
H,1,r2,2,90.,3,0.,0
H,1,r3,2,90.,3,180.,0
F,1,r4,2,90.,3,180.,0
O,1,r32,2,90.,3,0.,0
B,1,r42,2,90.,3,0.,0
H,1,r52,2,90.,3,0.,0

r1=1.21578141
r2=2.38449788
r3=1.74423587
r4=2.67909604
r32=4.73123328
r42=5.94708925
r52=7.11391238

HBO:HBO:HCN
MP2= -294.35472794

O
X,1,1.
B,1,r1,2,90.
H,1,r2,2,90.,3,0.,0
H,1,r3,2,90.,3,180.,0
C,1,r4,2,90.,3,180.,0
N,1,r5,2,90.,3,180.,0
O,1,r32,2,90.,3,0.,0
B,1,r42,2,90.,3,0.,0
H,1,r52,2,90.,3,0.,0

r1=1.21691834
r2=2.38592544
r3=2.03792626
r4=3.11109967
r5=4.27844689
r32=4.7493885
r42=5.96521939
r52=7.13210566

HBO:HBO:HCl
MP2= -661.40993648

O
X,1,1.
B,1,r1,2,90.
H,1,r2,2,90.,3,0.,0
H,1,r3,2,90.,3,180.,0
Cl,1,r4,2,90.,3,180.,0
O,1,r32,2,90.,3,0.,0
B,1,r42,2,90.,3,0.,0
H,1,r52,2,90.,3,0.,0

r1=1.21674
r2=2.38561956
r3=1.90365751

HBO:HBO:ClF
MP2= -760.45662863

r4=3.19180147
r32=4.75151449
r42=5.96729212
r52=7.1341807
O
X,1,1.
B,1,r1,2,90.
H,1,r2,2,90.,3,0.,0
Cl,1,r3,2,90.,3,180.,0
F,1,r4,2,90.,3,180.,0
O,1,r32,2,90.,3,0.,0
B,1,r42,2,90.,3,0.,0
H,1,r52,2,90.,3,0.,0

HBO:HBO:HBO
MP2= -301.63165745

r1=1.21657773
r2=2.38546857
r3=2.55536337
r4=4.20767407
r32=4.7613563
r42=5.97708378
r52=7.14391531
O
X,1,1.
B,1,r1,2,90.
H,1,r2,2,90.,3,0.,0
H,1,r3,2,90.,3,180.,0
B,1,r4,2,90.,3,180.,0
O,1,r5,2,90.,3,180.,0
O,1,r32,2,90.,3,0.,0
B,1,r42,2,90.,3,0.,0
H,1,r52,2,90.,3,0.,0

HNC:HBO:LiH
MP2= -201.81973243

r1=1.2168751
r2=2.3859201
r3=2.39724902
r4=3.56670882
r5=4.78339918
r32=4.78088769
r42=5.99657266
r52=7.16345503

O
X,1,1.
B,1,r1,2,90.
H,1,r2,2,90.,3,0.,0
Li,1,r3,2,90.,3,180.,0
H,1,r4,2,90.,3,180.,0
C,1,r32,2,90.,3,0.,0
N,1,r42,2,90.,3,0.,0
H,1,r52,2,90.,3,0.,0

HNC:HBO:HNC
MP2= -287.02137487

r1=1.21762396
r2=2.38741786
r3=1.93100132
r4=3.56496499
r32=4.9554864
r42=6.12979471
r52=7.12879608

O
X,1,1.
B,1,r1,2,90.
H,1,r2,2,90.,3,0.,0
H,1,r3,2,90.,3,180.,0
N,1,r4,2,90.,3,180.,0
C,1,r5,2,90.,3,180.,0
C,1,r32,2,90.,3,0.,0
N,1,r42,2,90.,3,0.,0
H,1,r52,2,90.,3,0.,0

r1=1.21729945
r2=2.38664767
r3=1.80251756
r4=2.81590603
r5=3.99206936
r32=5.02650105
r42=6.20134054
r52=7.2000506

HNC:HBO:HF
MP2= -294.12977362

O
X,1,1.
B,1,r1,2,90.
H,1,r2,2,90.,3,0.,0
H,1,r3,2,90.,3,180.,0
F,1,r4,2,90.,3,180.,0
C,1,r32,2,90.,3,0.,0
N,1,r42,2,90.,3,0.,0
H,1,r52,2,90.,3,0.,0

r1=1.21607434
r2=2.38519322
r3=1.74431418
r4=2.67928851
r32=5.03758485
r42=6.21254955
r52=7.21117065

HNC:HBO:HCN
MP2= -287.04435948

O
X,1,1.
B,1,r1,2,90.
H,1,r2,2,90.,3,0.,0
H,1,r3,2,90.,3,180.,0
C,1,r4,2,90.,3,180.,0
N,1,r5,2,90.,3,180.,0
C,1,r32,2,90.,3,0.,0
N,1,r42,2,90.,3,0.,0
H,1,r52,2,90.,3,0.,0

r1=1.21721589
r2=2.38658546
r3=2.0379331
r4=3.11108957
r5=4.27847943
r32=5.05701679
r42=6.23208816
r52=7.23069269

HNC:HBO:HCl
MP2= -654.09952802

O
X,1,1.
B,1,r1,2,90.
H,1,r2,2,90.,3,0.,0
H,1,r3,2,90.,3,180.,0
Cl,1,r4,2,90.,3,180.,0
C,1,r32,2,90.,3,0.,0
N,1,r42,2,90.,3,0.,0
H,1,r52,2,90.,3,0.,0

r1=1.21704368
r2=2.38626395

r3=1.90376601
r4=3.19187762
r32=5.06072191
r42=6.2358433
r52=7.23433516

HNC:HBO:ClF
MP2= -753.14624276

O
X,1,1.
B,1,r1,2,90.
H,1,r2,2,90.,3,0.,0
Cl,1,r3,2,90.,3,180.,0
F,1,r4,2,90.,3,180.,0
C,1,r32,2,90.,3,0.,0
N,1,r42,2,90.,3,0.,0
H,1,r52,2,90.,3,0.,0

r1=1.21688695
r2=2.38610517
r3=2.55479335
r4=4.20723811
r32=5.06976575
r42=6.24496008
r52=7.24347628

HNC:HBO:HBO
MP2= -294.32132066

O
X,1,1.
B,1,r1,2,90.
H,1,r2,2,90.,3,0.,0
H,1,r3,2,90.,3,180.,0
B,1,r4,2,90.,3,180.,0
O,1,r5,2,90.,3,180.,0
C,1,r32,2,90.,3,0.,0
N,1,r42,2,90.,3,0.,0
H,1,r52,2,90.,3,0.,0

r1=1.2171905
r2=2.38654347
r3=2.39700192
r4=3.56640297
r5=4.78318641
r32=5.09347925
r42=6.26877875
r52=7.26727506

HCN:HBO:LiH
MP2= -201.84816741

O
X,1,1.
B,1,r1,2,90.
H,1,r2,2,90.,3,0.,0
Li,1,r3,2,90.,3,180.,0
H,1,r4,2,90.,3,180.,0

HCN:HBO:HNC
MP2= -287.04987782

N,1,r32,2,90.,3,0.,0
C,1,r42,2,90.,3,0.,0
H,1,r52,2,90.,3,0.,0

r1=1.21741039
r2=2.38663272
r3=1.93169037
r4=3.56554732
r32=4.80238959
r42=5.96819101
r52=7.03505975

O
X,1,1.
B,1,r1,2,90.
H,1,r2,2,90.,3,0.,0
H,1,r3,2,90.,3,180.,0
N,1,r4,2,90.,3,180.,0
C,1,r5,2,90.,3,180.,0
N,1,r32,2,90.,3,0.,0
C,1,r42,2,90.,3,0.,0
H,1,r52,2,90.,3,0.,0

HCN:HBO:HF
MP2= -294.15825505

r1=1.2170972
r2=2.38606266
r3=1.80349361
r4=2.81678967
r5=3.99298683
r32=4.86724972
r42=6.03332101
r52=7.09997362

O
X,1,1.
B,1,r1,2,90.
H,1,r2,2,90.,3,0.,0
H,1,r3,2,90.,3,180.,0
F,1,r4,2,90.,3,180.,0
N,1,r32,2,90.,3,0.,0
C,1,r42,2,90.,3,0.,0
H,1,r52,2,90.,3,0.,0

HCN:HBO:HCN
MP2= -287.07283487

r1=1.21587632
r2=2.38462562
r3=1.74520119
r4=2.68011031
r32=4.87938115
r42=6.04549767
r52=7.11209327

O
X,1,1.
B,1,r1,2,90.

H,1,r2,2,90.,3,0.,0
H,1,r3,2,90.,3,180.,0
C,1,r4,2,90.,3,180.,0
N,1,r5,2,90.,3,180.,0
N,1,r32,2,90.,3,0.,0
C,1,r42,2,90.,3,0.,0
H,1,r52,2,90.,3,0.,0

r1=1.21701897
r2=2.38605565
r3=2.03924783
r4=3.11236107
r5=4.27972623
r32=4.89631814
r42=6.06246637
r52=7.1290504

HCN:HBO:HCl
MP2= -654.12802259

O
X,1,1.
B,1,r1,2,90.
H,1,r2,2,90.,3,0.,0
H,1,r3,2,90.,3,180.,0
Cl,1,r4,2,90.,3,180.,0
N,1,r32,2,90.,3,0.,0
C,1,r42,2,90.,3,0.,0
H,1,r52,2,90.,3,0.,0

r1=1.21685728
r2=2.38578258
r3=1.90495982
r4=3.19297546
r32=4.90005725
r42=6.06624239
r52=7.13279727

HCN:HBO:ClF
MP2= -753.17473527

O
X,1,1.
B,1,r1,2,90.
H,1,r2,2,90.,3,0.,0
Cl,1,r3,2,90.,3,180.,0
F,1,r4,2,90.,3,180.,0
N,1,r32,2,90.,3,0.,0
C,1,r42,2,90.,3,0.,0
H,1,r52,2,90.,3,0.,0

r1=1.21669259
r2=2.38562178
r3=2.55718315
r4=4.20969403
r32=4.90974286
r42=6.07595873
r52=7.14248335

HCN:HBO:HBO
MP2= -294.34980108

O
X,1,1.
B,1,r1,2,90.
H,1,r2,2,90.,3,0.,0
H,1,r3,2,90.,3,180.,0
B,1,r4,2,90.,3,180.,0
O,1,r5,2,90.,3,180.,0
N,1,r32,2,90.,3,0.,0
C,1,r42,2,90.,3,0.,0
H,1,r52,2,90.,3,0.,0

r1=1.21700122
r2=2.38609741
r3=2.3982091
r4=3.56759918
r5=4.78430885
r32=4.92901966
r42=6.09527291
r52=7.16178362

HF:HBO:LiH
MP2= -208.92665905

O,0.1174297,0.,0.
B,1.3340469367,0.,0.
H,2.5004983357,0.,0.
Li,-1.8195883363,0.,0.
H,-3.451735992,0.,0.
F,4.7951982639,0.,0.
H,5.7185077119,0.,0.

HF:HBO:HNC
MP2= -294.12890869

O,0.1089967437,0.,0.
B,1.3254448886,0.,0.
H,2.4922405831,0.,0.
H,-1.7042926676,0.,0.
N,-2.7167235003,0.,0.
C,-3.8929601267,0.,0.
F,4.8428058022,0.,0.
H,5.765784037,0.,0.

HF:HBO:HF
MP2= -301.23741252

O,0.123305038,0.,0.
B,1.3385896742,0.,0.
H,2.505379229,0.,0.
H,-1.6304184022,0.,0.
F,-2.5646461048,0.,0.
F,4.8663046803,0.,0.
H,5.7892851556,0.,0.

HF:HBO:HCN
MP2= -294.15206137

O,0.110447329,0.,0.
B,1.3268276,0.,0.
H,2.4938976736,0.,0.
H,-1.9398612551,0.,0.
C,-3.0125145154,0.,0.
N,-4.179859351,0.,0.
F,4.871811167,0.,0.
H,5.794655552,0.,0.

HF:HBO:HCl
MP2= -661.20730659

O,0.1265086965,0.,0.
B,1.3427251519,0.,0.
H,2.509684604,0.,0.
H,-1.7917644834,0.,0.
Cl,-3.078908917,0.,0.
F,4.8865920885,0.,0.
H,5.8093920695,0.,0.

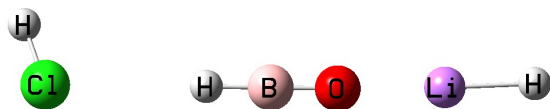
HF:HBO:ClF
MP2= -760.25409481

O,0.1249976164,0.,0.
B,1.3410792347,0.,0.
H,2.5081280039,0.,0.
Cl,-2.4414923081,0.,0.
F,-4.0929759607,0.,0.
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HF:HBO:HBO
MP2= -301.42923917

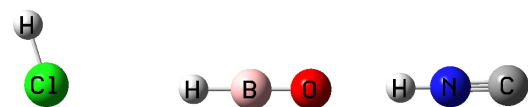
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H,2.4972683065,0.,0.
H,-2.2973573275,0.,0.
B,-3.4666043435,0.,0.
O,-4.6832421199,0.,0.
F,4.9015456482,0.,0.
H,5.8242595268,0.,0.

HCl:HBO:LiH
MP2= -568.89852844



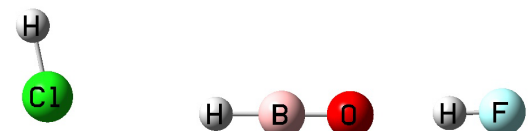
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B,0.,-0.039759834,-1.3381001004
H,0.,-0.0482208571,-0.171036091
Li,0.,0.0428058063,-4.4934467261
H,0.,0.1595487374,-6.119957538
Cl,0.,-0.0877981066,2.7499610793
H,0.,1.1113845055,3.186098797

HCl:HBO:HNC
MP2= -654.10127486



O,0.,0.0401261979,-1.2163534115
B,0.,0.0687666089,-0.000648683
H,0.,0.092913076,1.1663668681
H,0.,-0.0280087475,-3.037636183
N,0.,-0.0728516985,-4.0483315728
C,0.,-0.1264011289,-5.2233919753
Cl,0.,0.0690915115,4.1555966266

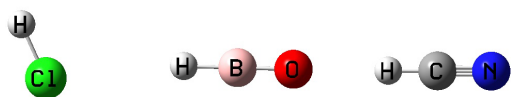
HCl:HBO:HF
MP2= -661.20989497



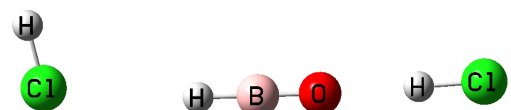
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O,0.0280254597,0.,-1.7918861237
B,0.1021756305,0.,-0.5792882057
H,0.1695976697,0.,0.5858407542
H,-0.1135989067,0.,-3.5476415116
F,-0.1948697192,0.,-4.4777483589
Cl,0.06346214,0.,3.5864454986
H,-1.1647922739,0.,3.9311929471

HCl:HBO:HCN
MP2= -654.12459800

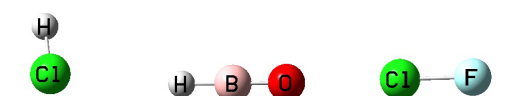
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H,0.,-0.1083178892,1.2599559383
H,0.,-0.0054924091,-3.1827658999



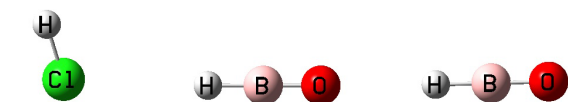
HCl:HBO:HCl
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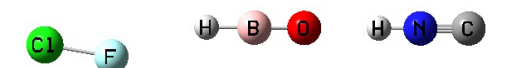
HCl:HBO:ClF
MP2= -1120.22678889



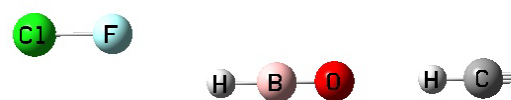
HCl:HBO:HBO
MP2= -661.40197979



ClF:HBO:HNC
MP2= -753.14853145



ClF:HBO:HCN
MP2= -753.17185551



ClF:HBO:ClF
MP2= -1219.27402864

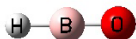


ClF:HBO:HBO

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O,0.,0.0604954567,-0.8741568144
B,0.,0.1225507546,0.3401016277
H,0.,0.1785197791,1.5061005057
H,0.,-0.0995910381,-2.7979100271
Cl,0.,-0.2176961633,-4.0788395351
Cl,0.,0.0397188252,4.5234184393
H,0.,-1.1939976142,4.847819804
O,0.070360232,0.,-0.2981327375
B,0.1316766772,0.,0.9160312135
H,0.186777774,0.,2.0821493306
Cl,-0.1042047887,0.,-2.8685691182
F,-0.2190979999,0.,-4.5152864074
Cl,0.0212976325,0.,5.108201203
H,-1.2168095272,0.,5.415226516
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Cl,0.0437278367,0.,4.4808325741
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B,0.,0.4131192931,-0.8269432404
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C,0.,-0.0886783082,-5.1468160335
N,0.,-0.2216586922,-6.3065337809
F,0.,-0.2516121911,2.6898613407
Cl,0.,-0.0770845617,4.3217521885
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Cl,-0.0240964388,0.,5.1911245103
O,0.,0.2764402969,-1.9015987565

MP2= -760.44923724



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B,0.,-0.0942829861,-5.475688207
O,0.,-0.2161241301,-6.686101867
F,0.,-0.230224353,2.85645149
Cl,0.,-0.1018431859,4.4922429393

Table S2. MP2/aug'-cc-pVTZ binding energies of ternary complexes, binary complexes isolated and in ternary complexes, and enhanced binding energies of ternary complexes X:HBO:Z (kJ/mol) for fixed Z as a function of X^a

X:HBO:Z	δE (X:HBO:Z)	δE (ternary X:HBO)	δE (ternary HBO:Z)	δE (binary X:HBO)	δE (binary HBO:Z)	$\delta(\delta E)$
HCl:HBO:LiH	-75.91	-6.08	-72.38	-3.53	-69.83	-2.55
HF:HBO:LiH	-81.66	-11.83	-75.42	-6.24	-69.83	-5.59
HCN:HBO:LiH	-87.33	-17.50	-78.68	-8.64	-69.83	-8.85
HNC:HBO:LiH	-88.71	-18.88	-78.89	-9.82	-69.83	-9.06
HBO:HBO:LiH	-89.16	-19.33	-79.04	-10.12	-69.83	-9.21
LiH:HBO:LiH	-104.22	-34.39	-87.52	-16.69	-69.83	-17.69
CIF:HBO:HNC	-39.01	-4.62	-35.76	-3.25	-34.38	-1.38
HCl:HBO:HNC	-39.30	-4.92	-35.77	-3.53	-34.38	-1.39
HF:HBO:HNC	-43.75	-9.36	-37.51	-6.24	-34.38	-3.13
HCN:HBO:HNC	-48.00	-13.62	-39.36	-8.64	-34.38	-4.97
HNC:HBO:HNC	-49.20	-14.82	-39.39	-9.82	-34.38	-5.00
HBO:HBO:HNC	-49.72	-15.33	-39.60	-10.12	-34.38	-5.21
LiH:HBO:HNC	-61.02	-26.64	-44.33	-16.69	-34.38	-9.94
HCl:HBO:HF	-36.70	-4.65	-33.17	-3.53	-32.05	-1.12
HF:HBO:HF	-40.84	-8.79	-34.60	-6.24	-32.05	-2.56
HCN:HBO:HF	-44.76	-12.71	-36.12	-8.64	-32.05	-4.07
HNC:HBO:HF	-46.02	-13.97	-36.20	-9.82	-32.05	-4.16
HBO:HBO:HF	-46.42	-14.38	-36.30	-10.12	-32.05	-4.26
LiH:HBO:HF	-56.87	-24.82	-40.17	-16.69	-32.05	-8.13
CIF:HBO:HCN	-24.21	-4.18	-20.96	-3.25	-20.03	-0.93
HCl:HBO:HCN	-24.50	-4.47	-20.97	-3.53	-20.03	-0.94
HF:HBO:HCN	-28.50	-8.47	-22.26	-6.24	-20.03	-2.23
HCN:HBO:HCN	-32.24	-12.21	-23.59	-8.64	-20.03	-3.56
HNC:HBO:HCN	-33.51	-13.48	-23.70	-9.82	-20.03	-3.67
HBO:HBO:HCN	-33.78	-13.75	-23.66	-10.12	-20.03	-3.63
LiH:HBO:HCN	-43.89	-23.86	-27.19	-16.69	-20.03	-7.16
HCl:HBO:HCl	-26.12	-4.40	-22.59	-3.53	-21.72	-0.87
HF:HBO:HCl	-29.90	-8.18	-23.67	-6.24	-21.72	-1.95
HCN:HBO:HCl	-33.49	-11.77	-24.85	-8.64	-21.72	-3.13
HNC:HBO:HCl	-34.72	-12.99	-24.90	-9.82	-21.72	-3.18
HBO:HBO:HCl	-35.09	-13.37	-24.97	-10.12	-21.72	-3.25
LiH:HBO:HCl	-44.68	-22.96	-27.98	-16.69	-21.72	-6.26
CIF:HBO:CIF	-24.46	-3.93	-21.21	-3.25	-20.53	-0.68
HCl:HBO:CIF	-24.80	-4.27	-21.26	-3.53	-20.53	-0.74
HF:HBO:CIF	-28.38	-7.85	-22.14	-6.24	-20.53	-1.62
HCN:HBO:CIF	-31.77	-11.24	-23.13	-8.64	-20.53	-2.60
HNC:HBO:CIF	-33.00	-12.47	-23.18	-9.82	-20.53	-2.66
HBO:HBO:CIF	-33.31	-12.78	-23.19	-10.12	-20.53	-2.67
LiH:HBO:CIF	-42.45	-21.92	-25.76	-16.69	-20.53	-5.23

Table S2, continued

CIF:HBO:HBO	-13.91	-3.79	-10.66	-3.25	-10.12	-0.54
HCl:HBO:HBO	-14.20	-4.08	-10.67	-3.53	-10.12	-0.55
HF:HBO:HBO	-17.66	-7.54	-11.42	-6.24	-10.12	-1.31
HCN:HBO:HBO	-20.84	-10.72	-12.20	-8.64	-10.12	-2.08
HNC:HBO:HBO	-22.11	-11.99	-12.29	-9.82	-10.12	-2.17
HBO:HBO:HBO	-22.29	-12.17	-12.17	-10.12	-10.12	-2.05
LiH:HBO:HBO	-30.99	-20.87	-14.29	-16.69	-10.12	-4.17

Table S3. Spin-spin coupling constants (Hz) for the B-H...A interaction in complexes X:HBO:Z for fixed X as a function of Z, with A the atom of X interacting with B-H

LiH:HBO:Z: $^1J(\text{B-H})$, $^2dJ(\text{B-H})$, $^1dJ(\text{H-H})$

LiH:HBO:LiH

PSO	DSO	FC	SD	J	
-0.2	0.5	269.8	0.8	270.8	1J
0.0	0.2	12.3	0.1	12.5	2dJ
-1.5	1.7	-2.2	-0.1	-2.0	1dJ

LiH:HBO:HNC

-0.3	0.5	262.3	0.7	263.2	1J
0.0	0.2	10.0	0.1	10.2	2dJ
-1.4	1.6	-2.0	-0.1	-1.8	1dJ

LiH:HBO:HF

-0.3	0.5	262.3	0.7	263.2	1J
0.0	0.2	9.7	0.1	9.9	2dJ
-1.4	1.6	-2.0	-0.1	-1.8	1dJ

LiH:HBO:HCN

-0.3	0.5	258.2	0.7	259.0	1J
0.0	0.2	9.2	0.1	9.4	2dJ
-1.3	1.6	-1.9	-0.1	-1.7	1dJ

LiH:HBO:HCl

-0.3	0.5	259.1	0.7	259.9	1J
0.0	0.2	9.2	0.1	9.4	2dJ
-1.3	1.6	-1.9	-0.1	-1.7	1dJ

LiH:HBO:ClF

-0.3	0.5	258.0	0.7	258.8	1J
0.0	0.2	8.9	0.1	9.1	2dJ
-1.3	1.6	-1.8	-0.1	-1.6	1dJ

LiH:HBO:HBO

-0.3	0.5	254.0	0.6	254.8	1J
0.0	0.2	8.4	0.1	8.5	2dJ
-1.3	1.5	-1.8	0.0	-1.6	1dJ

HBO:HBO:Z ¹J(B-H), ^{2h}J(B-O), ^{1h}J(H-O)

HBO:HBO:LiH

PSO	DSO	FC	SD	J	
-0.4	0.6	267.9	0.7	268.7	1J
0.0	0.0	-8.8	0.0	-8.8	2hJ
0.4	-0.3	2.0	-0.2	1.9	1hJ

HBO:HBO:HNC

-0.4	0.6	259.4	0.6	260.2	1J
0.0	0.0	-7.1	0.0	-7.2	2hJ
0.3	-0.3	1.4	-0.2	1.3	1hJ

HBO:HBO:HF

-0.4	0.6	259.2	0.6	260.0	1J
0.0	0.0	-6.9	0.0	-6.9	2hJ
0.3	-0.3	1.3	-0.2	1.2	1hJ

HBO:HBO:HCN

-0.4	0.6	255.3	0.6	256.1	1J
0.0	0.0	-6.5	0.0	-6.6	2hJ
0.3	-0.3	1.2	-0.2	1.1	1hJ

HBO:HBO:HCl

-0.4	0.6	256.0	0.6	256.7	1J
0.0	0.0	-6.5	0.0	-6.5	2hJ
0.3	-0.3	1.2	-0.2	1.0	1hJ

HBO:HBO:ClF

-0.4	0.6	254.8	0.6	255.5	1J
0.0	0.0	-6.3	0.0	-6.3	2hJ
0.3	-0.3	1.1	-0.2	1.0	1hJ

HBO:HBO:HBO

-0.4	0.6	251.1	0.6	251.9	1J
0.0	0.0	-5.9	0.0	-6.0	2hJ
0.3	-0.2	1.0	-0.2	0.8	1hJ

HNC:HBO:Z $^1J(B-H)$, $^2hJ(B-C)$, $^1hJ(H-C)$

HNC:HBO:LiH

PSO	DSO	FC	SD	J	
-0.4	0.5	267.3	0.7	268.1	1J
0.0	0.1	15.6	0.0	15.7	2hJ
-0.2	0.5	-3.4	0.2	-3.0	1hJ

HNC:HBO:HNC

-0.4	0.5	258.8	0.6	259.6	1J
0.0	0.1	12.7	0.0	12.8	2hJ
-0.2	0.4	-2.5	0.2	-2.1	1hJ

HNC:HBO:HF

-0.4	0.5	258.7	0.6	259.5	1J
0.0	0.1	12.3	0.0	12.3	2hJ
-0.2	0.4	-2.4	0.2	-1.9	1hJ

HNC:HBO:HCN

-0.4	0.5	254.8	0.6	255.5	1J
0.0	0.1	11.6	0.0	11.7	2hJ
-0.2	0.4	-2.2	0.2	-1.8	1hJ

HNC:HBO:HCl

-0.4	0.5	255.4	0.6	256.1	1J
0.0	0.1	11.5	0.0	11.6	2hJ
-0.2	0.4	-2.1	0.2	-1.7	1hJ

HNC:HBO:ClF

-0.4	0.5	254.3	0.6	255.1	1J
0.0	0.1	11.2	0.0	11.3	2hJ
-0.2	0.4	-2.0	0.2	-1.6	1hJ

HNC:HBO:HBO

-0.4	0.5	250.6	0.6	251.3	1J
0.0	0.1	10.5	0.0	10.5	2hJ
-0.2	0.4	-1.8	0.2	-1.4	1hJ

HCN:HBO:Z $^1J(\text{B-H})$, $^2hJ(\text{B-N})$, $^1hJ(\text{H-N})$

HCN:HBO:LiH

PSO	DSO	FC	SD	J	
-0.4	0.5	267.7	0.7	268.5	1J
0.0	0.0	-6.4	0.0	-6.4	2hJ
0.2	-0.2	1.4	-0.1	1.2	1hJ

HCN:HBO:HNC

-0.4	0.5	259.2	0.6	259.9	1J
0.0	0.0	-5.2	0.0	-5.3	2hJ
0.1	-0.2	1.0	-0.1	0.8	1hJ

HCN:HBO:HF

-0.4	0.5	259.0	0.6	259.8	1J
0.0	0.0	-5.0	0.0	-5.1	2hJ
0.1	-0.2	1.0	-0.1	0.8	1hJ

HCN:HBO:HCN

-0.4	0.5	255.1	0.6	255.8	1J
0.0	0.0	-4.8	0.0	-4.8	2hJ
0.1	-0.2	0.9	-0.1	0.7	1hJ

HCN:HBO:HCl

-0.4	0.5	255.7	0.6	256.5	1J
0.0	0.0	-4.7	0.0	-4.8	2hJ
0.1	-0.2	0.9	-0.1	0.7	1hJ

HCN:HBO:ClF

-0.4	0.6	254.6	0.6	255.3	1J
0.0	0.0	-4.6	0.0	-4.6	2hJ
0.1	-0.2	0.8	-0.1	0.6	1hJ

HCN:HBO:HBO

-0.4	0.5	250.9	0.6	251.6	1J
0.0	0.0	-4.3	0.0	-4.4	2hJ
0.1	-0.2	0.7	-0.1	0.6	1hJ

HF:HBO:Z $^1J(\text{B-H}), ^2hJ(\text{B-F}), ^1hJ(\text{H-F})$

HF:HBO:LiH

PSO	DSO	FC	SD	J	
-0.4	0.6	266.3	0.7	267.1	1J
0.1	0.2	35.8	0.1	36.2	2hJ
-0.2	1.5	-4.3	-0.6	-3.5	1hJ

HF:HBO:HNC

-0.4	0.6	257.6	0.6	258.3	1J
0.1	0.2	29.9	0.0	30.2	2hJ
-0.2	1.5	-2.1	-0.6	-1.5	1hJ

HF:HBO:HF

-0.4	0.6	257.4	0.6	258.2	1J
0.1	0.2	28.9	0.0	29.2	2hJ
-0.2	1.5	-1.9	-0.5	-1.2	1hJ

HF:HBO:HCN

-0.4	0.6	253.6	0.6	254.3	1J
0.1	0.2	27.2	0.0	27.5	2hJ
-0.2	1.4	-1.4	-0.5	-0.7	1hJ

HF:HBO:HCl

-0.4	0.6	254.1	0.6	254.8	1J
0.1	0.2	27.4	0.0	27.7	2hJ
-0.2	1.4	-1.4	-0.5	-0.7	1hJ

HF:HBO:ClF

-0.5	0.6	253.0	0.6	253.7	1J
0.1	0.2	26.4	0.0	26.7	2hJ
-0.2	1.4	-1.1	-0.5	-0.4	1hJ

HF:HBO:HBO

-0.4	0.6	249.5	0.6	250.1	1J
0.1	0.2	25.0	0.0	25.2	2hJ
-0.2	1.4	-0.7	-0.5	-0.1	1hJ

HCl:HBO:Z $^1J(\text{B-H}), ^2hJ(\text{B-Cl}), ^1hJ(\text{H-Cl})$
HCl:HBO:LiH

PSO	DSO	FC	SD	J	
-0.4	0.5	263.7	0.6	264.5	1J
0.0	0.0	2.3	0.0	2.3	2hJ
-0.2	0.1	-0.1	0.1	-0.2	1hJ
HCl:HBO:HNC					
-0.4	0.6	254.9	0.6	255.7	1J
0.0	0.0	1.8	0.0	1.8	2hJ
-0.2	0.1	0.0	0.1	-0.1	1hJ
HCl:HBO:HF					
-0.4	0.6	254.9	0.6	255.6	1J
0.0	0.0	1.7	0.0	1.8	2hJ
-0.2	0.1	0.0	0.1	-0.1	1hJ
HCl:HBO:HCN					
-0.4	0.6	251.0	0.6	251.7	1J
0.0	0.0	1.7	0.0	1.7	2hJ
-0.2	0.1	0.0	0.1	0.0	1hJ
HCl:HBO:HCl					
-0.4	0.6	251.5	0.6	252.2	1J
0.0	0.0	1.6	0.0	1.7	2hJ
-0.2	0.1	0.0	0.1	0.0	1hJ
HCl:HBO:ClF					
-0.4	0.6	250.5	0.6	251.2	1J
0.0	0.0	1.6	0.0	1.6	2hJ
-0.2	0.1	0.0	0.1	0.0	1hJ
HCl:HBO:HBO					
-0.4	0.6	247.0	0.5	247.7	1J
0.0	0.0	1.5	0.0	1.5	2hJ
-0.2	0.1	0.0	0.1	0.0	1hJ

CIF:HBO:Z $^1J(\text{B-H}), ^2J(\text{B-F}), ^1J(\text{H-F})$

CIF:HBO:HNC

PSO	DSO	FC	SD	J	
-0.5	0.6	255.2	0.6	255.9	1J
0.0	0.3	20.2	-0.1	20.4	2hJ
-0.3	2.0	1.5	-1.1	2.1	1hJ

CIF:HBO:HCN

-0.4	0.6	251.3	0.6	252.0	1J
0.0	0.3	18.9	-0.1	19.1	2hJ
0.0	1.9	2.4	-1.1	3.2	1hJ

CIF:HBO:CIF

-0.5	0.6	250.6	0.6	251.3	1J
0.0	0.3	18.7	-0.1	18.9	2hJ
0.0	2.0	2.3	-1.1	3.1	1hJ

CIF:HBO:HBO

-0.4	0.6	247.2	0.5	247.9	1J
0.0	0.3	18.0	-0.1	18.2	2hJ
0.2	1.9	2.6	-1.2	3.5	1hJ

Table S4. Spin-spin coupling constants (Hz) for the H-Li \cdots O, D-H \cdots O, and F-Cl \cdots O interactions in complexes X:HBO:Z for fixed Z as a function of X

X:HBO:LiH: $^1J(\text{Li-H})$, $^{2\text{li}}J(\text{H-O})$, $^{1\text{li}}J(\text{Li-O})$						
PSO	DSO	FC	SD	J		
LiH:HBO:LiH						
PSO	DSO	FC	SD	J		
-0.2	0.2	93.9	0.1	94.0	1J	
0.0	0.0	-2.7	0.0	-2.8	2liJ	
0.2	-0.1	-19.1	-0.1	-19.1	1liJ	
HBO:HBO:LiH						
-0.2	0.2	96.8	0.1	96.8	1J	
0.0	0.0	-2.9	0.0	-2.9	2liJ	
0.2	-0.1	-18.1	-0.1	-18.0	1liJ	
HNC:HBO:LiH						
-0.2	0.2	97.3	0.1	97.3	1J	
0.0	0.0	-2.9	0.0	-3.0	2liJ	
0.2	-0.1	-18.0	-0.1	-18.0	1liJ	
HCN:HBO:LiH						
-0.2	0.2	97.2	0.1	97.2	1J	
0.0	0.0	-2.9	0.0	-3.0	2liJ	
0.2	-0.1	-18.0	-0.1	-18.0	1liJ	
HF:HBO:LiH						
-0.2	0.2	98.3	0.1	98.4	1J	
0.0	0.0	-3.0	0.0	-3.1	2liJ	
0.2	-0.1	-17.5	-0.1	-17.5	1liJ	
HCl:HBO:LiH						
-0.2	0.2	99.5	0.1	99.6	1J	
0.0	0.0	-3.1	0.0	-3.2	2liJ	
0.2	-0.1	-17.2	-0.1	-17.2	1liJ	

X:HBO:HNC: $^1J(\text{N-H})$, $^{2h}J(\text{N-O})$, $^{1h}J(\text{H-O})$

	PSO	DSO	FC	SD	J
LiH:HBO:HNC					
	-0.1	-0.3	-114.2	-0.4	-115.0 1J
	-0.1	0.0	9.5	0.0	9.5 2hJ
	0.9	-0.6	6.6	-0.5	6.5 1hJ

HBO:HBO:HNC					
	-0.2	-0.3	-114.4	-0.4	-115.2 1J
	-0.1	0.0	8.8	0.0	8.8 2hJ
	0.9	-0.5	6.3	-0.5	6.2 1hJ

HNC:HBO:HNC					
	-0.2	-0.3	-114.4	-0.4	-115.2 1J
	-0.1	0.0	8.7	0.0	8.7 2hJ
	0.9	-0.5	6.3	-0.5	6.2 1hJ

HCN:HBO:HNC					
	-0.2	-0.3	-114.4	-0.4	-115.2 1J
	-0.1	0.0	8.7	0.0	8.7 2hJ
	0.9	-0.5	6.3	-0.5	6.2 1hJ

HF:HBO:HNC					
	-0.2	-0.3	-114.5	-0.4	-115.3 1J
	-0.1	0.0	8.4	0.0	8.4 2hJ
	0.8	-0.5	6.2	-0.5	6.0 1hJ

HCl:HBO:HNC					
	-0.2	-0.3	-114.6	-0.4	-115.4 1J
	-0.1	0.0	8.1	0.0	8.1 2hJ
	0.8	-0.5	6.1	-0.5	5.9 1hJ

ClF:HBO:HNC					
	-0.2	-0.3	-114.6	-0.4	-115.4 1J
	-0.1	0.0	8.1	0.0	8.1 2hJ
	0.8	-0.5	6.0	-0.5	5.9 1hJ

X:HBO:HF:	$^1J(\text{F-H}), ^2hJ(\text{F-O}), ^1hJ(\text{H-O})$				
	PSO	DSO	FC	SD	J
LiH:HBO:HF					
137.4	1.2	368.1	-1.7	505.0	1J
3.3	0.0	-25.7	-1.0	-23.5	2hJ
0.9	-0.7	7.5	-0.6	7.1	1hJ
HBO:HBO:HF					
140.5	1.2	365.8	-1.4	506.2	1J
3.1	0.0	-22.7	-1.0	-20.6	2hJ
0.9	-0.7	7.3	-0.6	7.0	1hJ
HNC:HBO:HF					
140.7	1.2	364.9	-1.4	505.5	1J
3.1	0.0	-22.4	-1.0	-20.4	2hJ
0.9	-0.7	7.4	-0.6	7.0	1hJ
HCN:HBO:HF					
140.7	1.2	365.3	-1.4	505.8	1J
3.1	0.0	-22.4	-1.0	-20.4	2hJ
0.9	-0.7	7.3	-0.6	7.0	1hJ
HF:HBO:HF					
142.0	1.2	364.1	-1.3	506.0	1J
3.0	0.0	-21.2	-1.0	-19.2	2hJ
0.9	-0.7	7.3	-0.6	6.9	1hJ
HCL:HBO:HF					
143.3	1.2	362.5	-1.2	505.9	1J
2.9	0.0	-19.9	-1.0	-18.0	2hJ
0.9	-0.7	7.2	-0.5	6.8	1hJ

X:HBO:HCN: $^1J(\text{C-H})$, $^{2h}J(\text{C-O})$, $^{1h}J(\text{H-O})$

	PSO	DSO	FC	SD	J
LiH:HBO:HCN					
	-0.7	0.5	253.9	0.5	254.2 1J
	0.0	0.0	-13.3	-0.1	-13.4 2hJ
	0.6	-0.4	4.6	-0.3	4.5 1hJ

HBO:HBO:HCN					
	-0.7	0.5	253.6	0.5	253.9 1J
	0.0	0.0	-12.2	-0.1	-12.2 2hJ
	0.6	-0.4	4.2	-0.3	4.0 1hJ

HNC:HBO:HCN					
	-0.7	0.5	253.6	0.5	253.9 1J
	0.0	0.0	-12.1	-0.1	-12.2 2hJ
	0.6	-0.4	4.2	-0.3	4.0 1hJ

HCN:HBO:HCN					
	-0.7	0.5	253.6	0.5	253.9 1J
	0.0	0.0	-12.1	-0.1	-12.2 2hJ
	0.6	-0.4	4.1	-0.3	4.0 1hJ

HF:HBO:HCN					
	-0.7	0.5	253.4	0.5	253.8 1J
	0.0	0.0	-11.7	-0.1	-11.7 2hJ
	0.6	-0.4	4.0	-0.3	3.8 1hJ

HCL:HBO:HCN					
	-0.7	0.5	253.3	0.5	253.6 1J
	0.0	0.0	-11.3	-0.1	-11.3 2hJ
	0.5	-0.4	3.8	-0.3	3.7 1hJ

CIF:HBO:HCN					
	-0.7	0.5	253.3	0.5	253.7 1J
	0.0	0.0	-11.3	-0.1	-11.3 2hJ
	0.5	-0.4	3.8	-0.3	3.7 1hJ

X:HBO:HCl: $^1J(\text{Cl-H}), ^2hJ(\text{Cl-O}), ^1hJ(\text{H-O})$					
	PSO	DSO	FC	SD	J
LiH:HBO:HCl					
	11.0	0.1	32.8	-0.2	43.7 1J
	0.4	0.0	-2.2	-0.2	-1.9 2hJ
	0.7	-0.6	10.5	-0.4	10.2 1hJ
HBO:HBO:HCl					
	11.4	0.0	31.9	-0.1	43.2 1J
	0.3	0.0	-1.7	-0.1	-1.5 2hJ
	0.6	-0.5	9.6	-0.4	9.3 1hJ
HNC:HBO:HCl					
	11.4	0.0	31.8	-0.1	43.1 1J
	0.3	0.0	-1.7	-0.1	-1.5 2hJ
	0.6	-0.5	9.7	-0.4	9.3 1hJ
HCN:HBO:HCl					
	11.4	0.0	31.8	-0.1	43.1 1J
	0.3	0.0	-1.7	-0.1	-1.5 2hJ
	0.6	-0.5	9.6	-0.4	9.3 1hJ
HF:HBO:HCl					
	11.5	0.0	31.4	-0.1	42.9 1J
	0.3	0.0	-1.5	-0.1	-1.3 2hJ
	0.6	-0.5	9.3	-0.4	9.0 1hJ
HCl:HBO:HCl					
	11.6	0.0	31.0	-0.1	42.6 1J
	0.3	0.0	-1.3	-0.1	-1.2 2hJ
	0.6	-0.5	9.0	-0.4	8.7 1hJ

X:HBO:ClF: $^1J(\text{F-Cl}), ^2J(\text{F-O}), ^1J(\text{Cl-O})$					
	PSO	DSO	FC	SD	J
LiH:HBO:ClF					
	593.1	0.1	-62.5	236.6	767.3 1J
	4.7	0.2	-7.1	-1.0	-3.2 2XJ
	-1.6	0.0	-34.4	-0.3	-36.3 1XJ
HBO:HBO:ClF					
	596.4	0.1	-67.0	237.9	767.4 1J
	4.2	0.2	-5.6	-0.9	-2.0 2XJ
	-1.5	0.0	-31.9	-0.2	-33.6 1XJ
HNC:HBO:ClF					
	596.8	0.1	-66.9	238.1	768.0 1J
	4.2	0.2	-5.4	-0.9	-1.9 2XJ
	-1.5	0.0	-31.9	-0.2	-33.6 1XJ
HCN:HBO:ClF					
	597.1	0.1	-66.9	238.2	768.5 1J
	4.2	0.2	-5.4	-0.9	-1.9 2XJ
	-1.4	0.0	-31.7	-0.2	-33.4 1XJ
HF:HBO:ClF					
	598.0	0.1	-68.7	238.5	767.9 1J
	4.0	0.2	-4.9	-0.9	-1.5 2XJ
	-1.4	0.0	-30.9	-0.2	-32.5 1XJ
HCl:HBO:ClF					
	599.2	0.1	-70.2	239.0	768.1 1J
	3.9	0.2	-4.4	-0.8	-1.1 2XJ
	-1.3	0.0	-30.0	-0.2	-31.5 1XJ
ClF:HBO:ClF					
	599.2	0.1	-70.2	238.9	768.0 1J
	3.9	0.2	-4.4	-0.8	-1.2 2XJ
	-1.3	0.0	-30.0	-0.2	-31.5 1XJ

X:HBO:HBO: $^1J(\text{B-H})$, $^{2h}J(\text{B-O})$, $^{1h}J(\text{H-O})$

	PSO	DSO	FC	SD	J
LiH:HBO:HBO					
	-0.4	0.6	249.0	0.6	249.7 1J
	0.0	0.0	-6.5	0.0	-6.6 2hJ
	0.3	-0.2	1.2	-0.2	1.1 1hJ

HBO:HBO:HBO					
	-0.4	0.6	248.2	0.6	248.9 1J
	0.0	0.0	-5.9	0.0	-5.9 2hJ
	0.3	-0.2	1.0	-0.2	0.8 1hJ

HNC:HBO:HBO					
	-0.4	0.6	248.1	0.6	248.8 1J
	0.0	0.0	-5.9	0.0	-5.9 2hJ
	0.3	-0.2	1.0	-0.2	0.8 1hJ

HCN:HBO:HBO					
	-0.4	0.6	248.1	0.6	248.8 1J
	0.0	0.0	-5.9	0.0	-5.9 2hJ
	0.3	-0.2	0.9	-0.2	0.8 1hJ

HF:HBO:HBO					
	-0.4	0.6	247.9	0.6	248.6 1J
	0.0	0.0	-5.6	0.0	-5.7 2hJ
	0.3	-0.2	0.9	-0.2	0.7 1hJ

HCl:HBO:HBO					
	-0.4	0.6	247.5	0.6	248.2 1J
	0.0	0.0	-5.4	0.0	-5.4 2hJ
	0.3	-0.2	0.8	-0.2	0.7 1hJ

ClF:HBO:HBO					
	-0.4	0.6	247.6	0.6	248.3 1J
	0.0	0.0	-5.4	0.0	-5.4 2hJ
	0.3	-0.2	0.8	-0.2	0.7 1hJ