Supporting Information

Systematic behaviour of electron redistribution on formation of halogen-bonded complexes B···XY, as determined via XY halogen nuclear quadrupole coupling constants

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Table S1. Electronic energy (hartree) and optimized geometry (Å) at MP2/aug-cc-pVTZ computational level and Nuclear quadrupole coupling constants (MHz) at MP2/aug-cc-pV5Z level for B:Cl_2 complexes.

Electronic energy (hartree) and optimized geometry (Å)	Nuclear quadrupole coupling constants (MHz)
Cl_2 MP2= -919.38707879 NIMAG= 0 Cl 0.000000000 0.000000000 0.000000000 Cl 0.000000000 0.000000000 1.998710000	1 Cl(35) aa= -111.0588 ba= -0.0000 ca= 0.0000 ab= -0.0000 bb= 55.5294 cb= 0.0000 ac= 0.0000 bc= 0.0000 cc= 55.5294 2 Cl(35) aa= -111.0588 ba= -0.0000 ca= 0.0000 ab= -0.0000 bb= 55.5294 cb= 0.0000 ac= 0.0000 bc= 0.0000 cc= 55.5294
N_2:Cl_2 MP2= -1028.75433916 NIMAG= 0 Cl 0.000000000 0.000000000 0.000000000 Cl 0.000000000 0.000000000 2.001606000 N 0.000000000 0.000000000 5.019688000 N 0.000000000 0.000000000 6.133849000	1 Cl(35) aa= -109.4710 ba= 0.0000 ca= 0.0000 ab= 0.0000 bb= 54.7355 cb= 0.0000 ac= 0.0000 bc= 0.0000 cc= 54.7355 2 Cl(35) aa= -111.5143 ba= 0.0000 ca= 0.0000 ab= 0.0000 bb= 55.7571 cb= 0.0000 ac= 0.0000 bc= 0.0000 cc= 55.7571
CO:Cl_2 MP2= -1032.53268343 NIMAG= 0 Cl 0.000000000 0.000000000 0.000000000 Cl 0.000000000 0.000000000 2.003755000 C 0.000000000 0.000000000 5.039269000 O 0.000000000 0.000000000 6.177353000	1 Cl(35) aa= -108.1335 ba= 0.0000 ca= 0.0000 ab= 0.0000 bb= 54.0668 cb= 0.0000 ac= 0.0000 bc= 0.0000 cc= 54.0668 2 Cl(35) aa= -112.0607 ba= 0.0000 ca= 0.0000 ab= 0.0000 bb= 56.0304 cb= 0.0000 ac= 0.0000 bc= 0.0000 cc= 56.0304
HC≡N:Cl_2 MP2= -1012.65225269 NIMAG= 0 Cl 0.000000000 0.000000000 0.000000000 Cl 0.000000000 0.000000000 2.007542000 N 0.000000000 0.000000000 4.829558000 C 0.000000000 0.000000000 5.995984000 H 0.000000000 0.000000000 7.061344000	1 Cl(35) aa= -105.7616 ba= 0.0000 ca= 0.0000 ab= 0.0000 bb= 52.8808 cb= 0.0000 ac= 0.0000 bc= 0.0000 cc= 52.8808 2 Cl(35) aa= -113.9249 ba= 0.0000 ca= 0.0000 ab= 0.0000 bb= 56.9624 cb= 0.0000 ac= 0.0000 bc= 0.0000 cc= 56.9624
H_2O:Cl_2 MP2= -995.72110781 NIMAG= 0 Cl 2.301695000 -0.055447000 -0.002729000 Cl 0.293657000 -0.075352000 0.003289000 O -2.480687000 -0.094500000 0.005730000 H -2.847687000 0.382240000 0.756779000 H -2.852364000 0.349174000 -0.763069000	1 Cl(35) aa= -106.0135 ba= 0.1960 ca= -2.0052 ab= 0.1960 bb= 52.9746 cb= 0.0024 ac= -2.0052 bc= 0.0024 cc= 53.0389 2 Cl(35) aa= -113.7109 ba= 0.1736 ca= -2.0383 ab= 0.1736 bb= 56.5523 cb= 0.0010 ac= -2.0383 bc= 0.0010 cc= 57.1586
H_2S:Cl_2 MP2= -1318.30106828 NIMAG= 0 Cl 2.858852000 -0.133180000 0.000388000 Cl 0.842491000 -0.122930000 -0.002742000 S -2.256846000 -0.046010000 -0.007132000 H -2.271934000 0.867893000 0.968676000 H -2.267070000 0.892674000 -0.959190000	1 Cl(35) aa= -105.3470 ba= 0.0146 ca= -3.7638 ab= 0.0146 bb= 52.6961 cb= 0.0003 ac= -3.7638 bc= 0.0003 cc= 52.6509 2 Cl(35) aa= -112.8401 ba= 0.0168 ca= -3.8770 ab= 0.0168 bb= 56.3017 cb= -0.0001 ac= -3.8770 bc= -0.0001 cc= 56.5384
HC≡CH:Cl_2 MP2= -996.55599495 NIMAG= 0 Cl 0.000000000 0.000000000 0.000000000 Cl 0.000000000 0.000000000 2.009685000 C 0.606854000 0.000000000 5.009140000 C -0.606854000 0.000000000 5.009140000 H 1.669335000 0.000000000 5.013174000 H -1.669335000 0.000000000 5.013174000	1 Cl(35) aa= -106.9660 ba= 0.0000 ca= -0.0000 ab= 0.0000 bb= 53.3555 cb= -0.0000 ac= -0.0000 bc= -0.0000 cc= 53.6105 2 Cl(35) aa= -112.2408 ba= 0.0000 ca= -0.0000 ab= 0.0000 bb= 55.2344 cb= -0.0000 ac= -0.0000 bc= -0.0000 cc= 57.0064
H_2C=CH_2:Cl_2 MP2= -997.79772732 NIMAG= 0 Cl 0.000000000 0.000000000 0.000000000 Cl 0.000000000 0.000000000 2.018917000 C 0.668619000 0.000000000 4.911135000 C -0.668619000 0.000000000 4.911135000 H 1.229876000 0.924074000 4.912556000 H 1.229876000 -0.924074000 4.912556000 H -1.229876000 -0.924074000 4.912556000 H -1.229876000 0.924074000 4.912556000	1 Cl(35) aa= -104.9545 ba= -0.0000 ca= 0.0000 ab= -0.0000 bb= 52.3890 cb= -0.0000 ac= 0.0000 bc= -0.0000 cc= 52.5655 2 Cl(35) aa= -112.3703 ba= -0.0000 ca= 0.0000 ab= -0.0000 bb= 55.5091 cb= -0.0000 ac= 0.0000 bc= -0.0000 cc= 56.8613

$PH_3:Cl_2$
MP2= -1262.05385212 NIMAG= 0

Cl	0.000000000	0.000000000	0.000000000
Cl	0.000000000	0.000000000	2.024610000
P	0.000000000	0.000000000	5.074901000
H	1.200580000	0.000000000	5.814908000
H	-0.600290000	1.039733000	5.814908000
H	-0.600290000	-1.039733000	5.814908000

1 Cl(35)
aa= -103.5204 ba= 0.0000 ca= -0.0000
ab= 0.0000 bb= 51.7602 cb= 0.0000
ac= -0.0000 bc= 0.0000 cc= 51.7602
2 Cl(35)
aa= -112.9623 ba= 0.0000 ca= -0.0000
ab= 0.0000 bb= 56.4811 cb= -0.0000
ac= -0.0000 bc= -0.0000 cc= 56.4811

$NH_3:Cl_2$
MP2= -975.85634482 NIMAG= 0

Cl	0.000000000	0.000000000	0.000000000
Cl	0.000000000	0.000000000	2.033659000
N	0.000000000	0.000000000	4.625494000
H	0.942783000	0.000000000	4.994526000
H	-0.471391000	0.816474000	4.994526000
H	-0.471391000	-0.816474000	4.994526000

1 Cl(35)
aa= -98.9668 ba= -0.0000 ca= 0.0000
ab= -0.0000 bb= 49.4834 cb= 0.0000
ac= 0.0000 bc= 0.0000 cc= 49.4834
2 Cl(35)
aa= -116.3364 ba= -0.0000 ca= 0.0000
ab= -0.0000 bb= 58.1682 cb= -0.0000
ac= 0.0000 bc= -0.0000 cc= 58.1682

$N(CH_3)_3:Cl_2$
MP2= -1093.51105006 NIMAG= ?

N	0.000000000	0.000000000	0.000000000
C	1.398104000	0.000000000	-0.421053000
C	-0.699052000	-1.210793000	-0.421053000
C	-0.699052000	1.210793000	-0.421053000
H	1.471170000	0.000000000	-1.514371000
H	-0.735585000	-1.274071000	-1.514371000
H	-0.735585000	1.274071000	-1.514371000
H	1.887131000	-0.885807000	-0.021851000
H	1.887131000	0.885807000	-0.021851000
H	-1.710697000	-1.191400000	-0.021851000
H	-0.176434000	-2.077207000	-0.021851000
H	-0.176434000	2.077207000	-0.021851000
H	-1.710697000	1.191400000	-0.021851000
Cl	0.000000000	0.000000000	2.141092000
Cl	0.000000000	0.000000000	4.317934000

14 Cl(35)
aa= -111.4753 ba= 0.0000 ca= -0.0000
ab= 0.0000 bb= 55.7377 cb= 0.0000
ac= -0.0000 bc= 0.0000 cc= 55.7377
15 Cl(35)
aa= -73.9581 ba= 0.0000 ca= -0.0000
ab= 0.0000 bb= 36.9790 cb= -0.0000
ac= -0.0000 bc= -0.0000 cc= 36.9790

Table S2. Electronic energy (hartree) and optimized geometry (Å) at MP2/aug-cc-pVTZ computational level and Nuclear quadrupole coupling constants (MHz) at MP2/aug-cc-pV5Z level for B:BrCl complexes.

Electronic energy (hartree) and optimized geometry (Å)				Nuclear quadrupole coupling constants (MHz)				
BrCl				1 Cl(35)				
MP2= -3032.38347008 NIMAG= 0				aa= -101.9564	ba= 0.0000	ca= 0.0000		
Cl	0.000000000	0.000000000	0.000000000	ab= 0.0000	bb= 50.9782	cb= 0.0000		
Br	0.000000000	0.000000000	2.138112000	ac= 0.0000	bc= 0.0000	cc= 50.9782		
				2 Br(79)				
				aa= 815.2387	ba= -0.0000	ca= -0.0000		
				ab= -0.0000	bb= -407.6193	cb= -0.0000		
				ac= -0.0000	bc= -0.0000	cc= -407.6193		
N_2:BrCl				1 Cl(35)				
MP2= -3141.75215627 NIMAG= 0				aa= -99.5149	ba= 0.0000	ca= 0.0000		
Cl	0.000000000	0.000000000	0.000000000	ab= 0.0000	bb= 49.7575	cb= 0.0000		
Br	0.000000000	0.000000000	2.142643000	ac= 0.0000	bc= 0.0000	cc= 49.7575		
N	0.000000000	0.000000000	5.121364000	2 Br(79)				
N	0.000000000	0.000000000	6.235556000	aa= 819.1248	ba= -0.0000	ca= -0.0000		
				ab= -0.0000	bb= -409.5624	cb= -0.0000		
				ac= -0.0000	bc= -0.0000	cc= -409.5624		
CO:BrCl				1 Cl(35)				
MP2= -3145.53149803 NIMAG= 0				aa= -96.6052	ba= 0.0000	ca= 0.0000		
Cl	0.000000000	0.000000000	0.000000000	ab= 0.0000	bb= 48.3026	cb= 0.0000		
Br	0.000000000	0.000000000	2.149705000	ac= 0.0000	bc= 0.0000	cc= 48.3026		
C	0.000000000	0.000000000	5.048326000	2 Br(79)				
O	0.000000000	0.000000000	6.185694000	aa= 824.8525	ba= -0.0000	ca= -0.0000		
				ab= -0.0000	bb= -412.4262	cb= -0.0000		
				ac= -0.0000	bc= -0.0000	cc= -412.4262		
HC≡N:BrCl				1 Cl(35)				
MP2= -3125.65238008 NIMAG= 0				aa= -93.9133	ba= 0.0000	ca= 0.0000		
Cl	0.000000000	0.000000000	0.000000000	ab= 0.0000	bb= 46.9567	cb= 0.0000		
Br	0.000000000	0.000000000	2.155510000	ac= 0.0000	bc= 0.0000	cc= 46.9567		
N	0.000000000	0.000000000	4.877593000	2 Br(79)				
C	0.000000000	0.000000000	6.043281000	aa= 842.0056	ba= -0.0000	ca= -0.0000		
H	0.000000000	0.000000000	7.109073000	ab= -0.0000	bb= -421.0028	cb= -0.0000		
				ac= -0.0000	bc= -0.0000	cc= -421.0028		
H_2O:BrCl				1 Cl(35)				
MP2= -3108.72089915 NIMAG= 0				aa= -94.5916	ba= -0.1147	ca= -1.4111		
Cl	2.373935000	-0.055829000	0.000378000	ab= -0.1147	bb= 47.2363	cb= -0.0009		
Br	0.219454000	-0.072431000	0.000892000	ac= -1.4111	bc= -0.0009	cc= 47.3553		
O	-2.478241000	-0.092830000	0.005411000	2 Br(79)				
H	-2.847774000	0.380241000	0.758324000	aa= 839.9373	ba= 0.8143	ca= 11.3162		
H	-2.852760000	0.346963000	-0.765004000	ab= 0.8143	bb= -416.5881	cb= -0.0025		
				ac= 11.3162	bc= -0.0025	cc= -423.3492		
H_2S:BrCl				1 Cl(35)				
MP2= -3431.30142776 NIMAG= 0				aa= -91.8377	ba= -0.0155	ca= -2.5363		
Cl	2.921495000	-0.136955000	-0.000182000	ab= -0.0155	bb= 45.8993	cb= -0.0001		
Br	0.747824000	-0.113605000	-0.003078000	ac= -2.5363	bc= -0.0001	cc= 45.9384		
S	-2.223396000	-0.047027000	-0.006208000	2 Br(79)				
H	-2.271033000	0.866561000	0.969687000	aa= 827.3866	ba= 0.1312	ca= 21.2630		
H	-2.269397000	0.889473000	-0.960219000	ab= 0.1312	bb= -411.5434	cb= -0.0070		
				ac= 21.2630	bc= -0.0070	cc= -415.8432		
HC≡CH:BrCl				1 Cl(35)				
MP2= -3109.55571003 NIMAG= 0				aa= -95.0656	ba= -0.0000	ca= -0.0000		
Cl	0.000000000	0.000000000	0.000000000	ab= -0.0000	bb= 47.3193	cb= -0.0000		
Br	0.000000000	0.000000000	2.158540000	ac= -0.0000	bc= -0.0000	cc= 47.7463		
C	0.607490000	0.000000000	5.065601000	2 Br(79)				
C	-0.607490000	0.000000000	5.065601000	aa= 823.4073	ba= 0.0000	ca= 0.0000		
H	1.670389000	0.000000000	5.077479000	ab= 0.0000	bb= -400.3865	cb= -0.0000		
H	-1.670389000	0.000000000	5.077479000	ac= 0.0000	bc= -0.0000	cc= -423.0208		
$H_2C=CH_2$:BrCl				1 Cl(35)				
MP2= -3110.79915384 NIMAG= 0				aa= -90.1340	ba= -0.0000	ca= -0.0000		
Cl	0.000000000	0.000000000	0.000000000	ab= -0.0000	bb= 44.8333	cb= 0.0000		
Br	0.000000000	0.000000000	2.180337000	ac= -0.0000	bc= 0.0000	cc= 45.3007		
C	0.671080000	0.000000000	4.922466000	2 Br(79)				
C	-0.671080000	0.000000000	4.922466000	aa= 818.1712	ba= 0.0000	ca= 0.0000		
H	1.231159000	0.924656000	4.929788000	ab= 0.0000	bb= -395.9148	cb= -0.0000		
H	1.231159000	-0.924656000	4.929788000	ac= 0.0000	bc= -0.0000	cc= -422.2564		
H	-1.231159000	-0.924656000	4.929788000					
H	-1.231159000	0.924656000	4.929788000					

PH_3:BrCl MP2= -3375.05674853 NIMAG= 0 Cl 0.000000000 0.000000000 0.000000000 Br 0.000000000 0.000000000 2.244830000 P 0.000000000 0.000000000 4.903886000 H 1.225145000 0.000000000 5.593465000 H -0.612573000 1.061007000 5.593465000 H -0.612573000 -1.061007000 5.593465000	1 Cl(35) aa= -76.8368 ba= 0.0000 ca= -0.0000 ab= 0.0000 bb= 38.4184 cb= -0.0000 ac= -0.0000 bc= -0.0000 cc= 38.4184 2 Br(79) aa= 797.3945 ba= 0.0000 ca= -0.0000 ab= 0.0000 bb= -398.6973 cb= 0.0000 ac= -0.0000 bc= 0.0000 cc= -398.6973
NH_3:BrCl MP2= -3088.86007270 NIMAG= 0 Cl 0.000000000 0.000000000 0.000000000 Br 0.000000000 0.000000000 2.202818000 N 0.000000000 0.000000000 4.671880000 H 0.946887000 0.000000000 5.030805000 H -0.473444000 0.820028000 5.030805000 H -0.473444000 -0.820028000 5.030805000	1 Cl(35) aa= -82.4839 ba= -0.0000 ca= 0.0000 ab= -0.0000 bb= 41.2420 cb= 0.0000 ac= 0.0000 bc= 0.0000 cc= 41.2420 2 Br(79) aa= 855.9153 ba= -0.0000 ca= -0.0000 ab= -0.0000 bb= -427.9576 cb= 0.0000 ac= -0.0000 bc= 0.0000 cc= -427.9576
$N(CH_3)_3$:BrCl MP2= -3206.51928934 NIMAG= ? N 0.000000000 0.000000000 0.000000000 C 1.395573000 0.000000000 -0.439491000 C -0.697786000 -1.208601000 -0.439491000 C -0.697786000 1.208601000 -0.439491000 H 1.452459000 0.000000000 -1.533389000 H -0.726229000 -1.257866000 -1.533389000 H -0.726229000 1.257866000 -1.533389000 H 1.889766000 -0.885792000 -0.046799000 H 1.889766000 0.885792000 -0.046799000 H -1.712001000 -1.193690000 -0.046799000 H -0.177765000 -2.079481000 -0.046799000 H -0.177765000 2.079481000 -0.046799000 H -1.712001000 1.193690000 -0.046799000 Br 0.000000000 0.000000000 2.227903000 Cl 0.000000000 0.000000000 4.517405000	14 Br(79) aa= 810.6299 ba= 0.0000 ca= 0.0000 ab= 0.0000 bb= -405.3150 cb= 0.0000 ac= 0.0000 bc= 0.0000 cc= -405.3150 15 Cl(35) aa= -66.9480 ba= 0.0000 ca= 0.0000 ab= 0.0000 bb= 33.4740 cb= 0.0000 ac= 0.0000 bc= 0.0000 cc= 33.4740

Table S3. Electronic energy (hartree) and optimized geometry (Å) at MP2/aug-cc-pVTZ computational level and Nuclear quadrupole coupling constants (MHz) at MP2/aug-cc-pV5Z level for B:Br_2 complexes.

Electronic energy (hartree) and optimized geometry (Å)				Nuclear quadrupole coupling constants (MHz)					
Br_2				1	Br(79)				
MP2= -5145.37847619 NIMAG= 0				aa=	755.2810	ba=	-0.0000	ca=	-0.0000
Br	0.000000000	0.000000000	0.000000000	ab=	-0.0000	bb=	-377.6405	cb=	-0.0000
Br	0.000000000	0.000000000	2.278606000	ac=	-0.0000	bc=	-0.0000	cc=	-377.6405
				2	Br(79)				
				aa=	755.2810	ba=	-0.0000	ca=	-0.0000
				ab=	-0.0000	bb=	-377.6405	cb=	-0.0000
				ac=	-0.0000	bc=	-0.0000	cc=	-377.6405
N_2:Br_2				1	Br(79)				
MP2= -5254.74693700 NIMAG= 0				aa=	738.8615	ba=	-0.0000	ca=	-0.0000
Br	0.000000000	0.000000000	0.000000000	ab=	-0.0000	bb=	-369.4308	cb=	-0.0000
Br	0.000000000	0.000000000	2.281937000	ac=	-0.0000	bc=	-0.0000	cc=	-369.4308
N	0.000000000	0.000000000	5.320253000	2	Br(79)				
N	0.000000000	0.000000000	6.434492000	aa=	758.9549	ba=	-0.0000	ca=	-0.0000
				ab=	-0.0000	bb=	-379.4775	cb=	-0.0000
				ac=	-0.0000	bc=	-0.0000	cc=	-379.4775
OC:Br_2				1	Br(79)				
MP2= -5258.52584909 NIMAG= 0				aa=	721.6681	ba=	-0.0000	ca=	-0.0000
Br	0.000000000	0.000000000	0.000000000	ab=	-0.0000	bb=	-360.8340	cb=	-0.0000
Br	0.000000000	0.000000000	2.287175000	ac=	-0.0000	bc=	-0.0000	cc=	-360.8340
C	0.000000000	0.000000000	5.274167000	2	Br(79)				
O	0.000000000	0.000000000	6.411877000	aa=	764.7375	ba=	-0.0000	ca=	-0.0000
				ab=	-0.0000	bb=	-382.3687	cb=	-0.0000
				ac=	-0.0000	bc=	-0.0000	cc=	-382.3687
HC≡N:Br_2				1	Br(79)				
MP2= -5238.64634281 NIMAG= 0				aa=	700.1694	ba=	-0.0000	ca=	-0.0000
Br	0.000000000	0.000000000	0.000000000	ab=	-0.0000	bb=	-350.0847	cb=	-0.0000
Br	0.000000000	0.000000000	2.292112000	ac=	-0.0000	bc=	-0.0000	cc=	-350.0847
N	0.000000000	0.000000000	5.080982000	2	Br(79)				
C	0.000000000	0.000000000	6.247072000	aa=	781.8886	ba=	-0.0000	ca=	-0.0000
H	0.000000000	0.000000000	7.312756000	ab=	-0.0000	bb=	-390.9443	cb=	-0.0000
				ac=	-0.0000	bc=	-0.0000	cc=	-390.9443
OH_2:Br_2				1	Br(79)				
MP2= -5221.71484739 NIMAG= 0				aa=	704.4998	ba=	-0.0000	ca=	9.1455
Br	1.702457000	0.010598000	0.000000000	ab=	-0.0000	bb=	-351.9060	cb=	0.0000
Br	-0.588855000	-0.027134000	0.000000000	ac=	9.1455	bc=	0.0000	cc=	-352.5938
O	-3.345403000	-0.063760000	0.000000000	2	Br(79)				
H	-3.721118000	0.390366000	0.761184000	aa=	779.6633	ba=	0.0000	ca=	9.0967
H	-3.721118000	0.390366000	-0.761184000	ab=	0.0000	bb=	-386.8732	cb=	-0.0000
				ac=	9.0967	bc=	-0.0000	cc=	-392.7901
SH_2:Br_2				1	Br(79)				
MP2= -5544.29539551 NIMAG= 0				aa=	689.0596	ba=	0.0000	ca=	18.9371
Br	3.053664000	-0.141448000	0.000000000	ab=	0.0000	bb=	-344.4778	cb=	-0.0000
Br	0.745978000	-0.126907000	0.000000000	ac=	18.9371	bc=	-0.0000	cc=	-344.5818
S	-2.297793000	-0.051598000	0.000000000	2	Br(79)				
H	-2.312181000	0.874744000	0.964600000	aa=	770.3338	ba=	-0.0000	ca=	19.6967
H	-2.312181000	0.874744000	-0.964600000	ab=	-0.0000	bb=	-383.4982	cb=	0.0000
				ac=	19.6967	bc=	0.0000	cc=	-386.8356
HC≡CH:Br_2				1	Br(79)				
MP2= -5222.55007313 NIMAG= 0				aa=	708.9793	ba=	-0.0000	ca=	0.0000
Br	0.000000000	0.000000000	0.000000000	ab=	-0.0000	bb=	-353.2791	cb=	0.0000
Br	0.000000000	0.000000000	2.295749000	ac=	0.0000	bc=	0.0000	cc=	-355.7002
C	0.607320000	0.000000000	5.260916000	2	Br(79)				
C	-0.607320000	0.000000000	5.260916000	aa=	764.8830	ba=	-0.0000	ca=	0.0000
H	1.670105000	0.000000000	5.270564000	ab=	-0.0000	bb=	-372.7853	cb=	-0.0000
H	-1.670105000	0.000000000	5.270564000	ac=	0.0000	bc=	-0.0000	cc=	-392.0978
H_2C=CH_2:Br_2				1	Br(79)				
MP2= -5223.79313927 NIMAG= 0				aa=	678.7927	ba=	-0.0000	ca=	0.0000
Br	0.000000000	0.000000000	0.000000000	ab=	-0.0000	bb=	-338.2243	cb=	-0.0000
Br	0.000000000	0.000000000	2.313937000	ac=	0.0000	bc=	-0.0000	cc=	-340.5684
C	0.670351000	0.000000000	5.128704000	2	Br(79)				
C	-0.670351000	0.000000000	5.128704000	aa=	763.1457	ba=	0.0000	ca=	0.0000
H	1.230636000	0.924609000	5.134239000	ab=	0.0000	bb=	-371.4853	cb=	-0.0000
H	1.230636000	-0.924609000	5.134239000	ac=	0.0000	bc=	-0.0000	cc=	-391.6604
H	-1.230636000	-0.924609000	5.134239000						
H	-1.230636000	0.924609000	5.134239000						

$PH_3:Br_2$	1 Br(79)
MP2= -5488.04964841 NIMAG= 0	aa= 627.6994 ba= -0.0000 ca= 0.0000
Br 0.000000000 0.000000000 0.000000000	ab= -0.0000 bb= -313.8497 cb= -0.0000
Br 0.000000000 0.000000000 2.344869000	ac= 0.0000 bc= -0.0000 cc= -313.8497
P 0.000000000 0.000000000 5.180578000	2 Br(79)
H 1.214216000 0.000000000 5.893235000	aa= 763.3548 ba= -0.0000 ca= -0.0000
H -0.607108000 1.051542000 5.893235000	ab= -0.0000 bb= -381.6774 cb= 0.0000
H -0.607108000 -1.051542000 5.893235000	ac= -0.0000 bc= 0.0000 cc= -381.6774
$NH_3:Br_2$	1 Br(79)
MP2= -5201.85272142 NIMAG= 0	aa= 625.2753 ba= 0.0000 ca= 0.0000
Br 0.000000000 0.000000000 0.000000000	ab= 0.0000 bb= -312.6377 cb= -0.0000
Br 0.000000000 0.000000000 2.332343000	ac= 0.0000 bc= -0.0000 cc= -312.6377
N 0.000000000 0.000000000 4.870394000	2 Br(79)
H 0.945931000 0.000000000 5.231538000	aa= 800.6192 ba= -0.0000 ca= 0.0000
H -0.472966000 0.819200000 5.231538000	ab= -0.0000 bb= -400.3096 cb= -0.0000
H -0.472966000 -0.819200000 5.231538000	ac= 0.0000 bc= -0.0000 cc= -400.3096
$N(CH_3)_3:Br_2$	14 Br(79)
MP2= -5319.51151490 NIMAG= ?	aa= 766.2723 ba= 0.0000 ca= 0.0000
N 0.000000000 0.000000000 0.000000000	ab= 0.0000 bb= -383.1362 cb= 0.0000
C 1.395177000 0.000000000 -0.435753000	ac= 0.0000 bc= 0.0000 cc= -383.1362
C -0.697588000 -1.208258000 -0.435753000	15 Br(79)
C -0.697588000 1.208258000 -0.435753000	aa= 503.1720 ba= 0.0000 ca= 0.0000
H 1.456490000 0.000000000 -1.529928000	ab= 0.0000 bb= -251.5860 cb= 0.0000
H -0.728245000 -1.261357000 -1.529928000	ac= 0.0000 bc= 0.0000 cc= -251.5860
H -0.728245000 1.261357000 -1.529928000	
H 1.889114000 -0.885798000 -0.042356000	
H 1.889114000 0.885798000 -0.042356000	
H -1.711681000 -1.193122000 -0.042356000	
H -0.177433000 -2.078920000 -0.042356000	
H -0.177433000 2.078920000 -0.042356000	
H -1.711681000 1.193122000 -0.042356000	
Br 0.000000000 0.000000000 2.258805000	
Br 0.000000000 0.000000000 4.681307000	

Table S4. Electronic energy (hartree) and optimized geometry (Å) at MP2/aug-cc-pVTZ computational level and Nuclear quadrupole coupling constants (MHz) at MP2/aug-cc-pV5Z level for B:ICl complexes.

Electronic energy (hartree) and optimized geometry (Å)	Nuclear quadrupole coupling constants (MHz)
ICl MP2= -754.58248119 NIMAG= 0 Cl 0.000000000 0.000000000 0.000000000 I 0.000000000 0.000000000 2.320932000	1 Cl(35) aa= -86.2163 ba= 0.0000 ca= 0.0000 ab= 0.0000 bb= 43.1081 cb= 0.0000 ac= 0.0000 bc= 0.0000 cc= 43.1081 2 I(127) aa= -2838.2660 ba= 0.0000 ca= 0.0000 ab= 0.0000 bb= 1419.1330 cb= 0.0000 ac= 0.0000 bc= 0.0000 cc= 1419.1330
N_2:ICl MP2= -863.95270543 NIMAG= 0 Cl 0.000000000 0.000000000 0.000000000 I 0.000000000 0.000000000 2.326771000 N 0.000000000 0.000000000 5.345317000 N 0.000000000 0.000000000 6.459555000	1 Cl(35) aa= -83.0507 ba= 0.0000 ca= 0.0000 ab= 0.0000 bb= 41.5254 cb= 0.0000 ac= 0.0000 bc= 0.0000 cc= 41.5254 2 I(127) aa= -2885.6417 ba= 0.0000 ca= 0.0000 ab= 0.0000 bb= 1442.8208 cb= 0.0000 ac= 0.0000 bc= 0.0000 cc= 1442.8208
CO:ICl MP2= -867.73338633 NIMAG= 0 Cl 0.000000000 0.000000000 0.000000000 I 0.000000000 0.000000000 2.340344000 C 0.000000000 0.000000000 5.192370000 O 0.000000000 0.000000000 6.329005000	1 Cl(35) aa= -77.8613 ba= 0.0000 ca= 0.0000 ab= 0.0000 bb= 38.9307 cb= 0.0000 ac= 0.0000 bc= 0.0000 cc= 38.9307 2 I(127) aa= -2916.2667 ba= 0.0000 ca= 0.0000 ab= 0.0000 bb= 1458.1333 cb= 0.0000 ac= 0.0000 bc= 0.0000 cc= 1458.1333
HC≡N:ICl MP2= -847.85576123 NIMAG= 0 Cl 0.000000000 0.000000000 0.000000000 I 0.000000000 0.000000000 2.347605000 N 0.000000000 0.000000000 5.052766000 C 0.000000000 0.000000000 6.217485000 H 0.000000000 0.000000000 7.283615000	1 Cl(35) aa= -75.4963 ba= 0.0000 ca= 0.0000 ab= 0.0000 bb= 37.7482 cb= 0.0000 ac= 0.0000 bc= 0.0000 cc= 37.7482 2 I(127) aa= -2984.9984 ba= 0.0000 ca= 0.0000 ab= 0.0000 bb= 1492.4992 cb= 0.0000 ac= 0.0000 bc= 0.0000 cc= 1492.4992
H_2O:ICl MP2= -830.92355086 NIMAG= 0 Cl 1.729388000 0.010816000 0.000207000 I -0.613387000 -0.028167000 -0.000351000 O -3.342882000 -0.061023000 -0.000374000 H -3.718716000 0.389716000 0.763830000 H -3.718058000 0.392401000 -0.763312000	1 Cl(35) aa= -77.5549 ba= -0.0160 ca= -1.2737 ab= -0.0160 bb= 38.6850 cb= -0.0001 ac= -1.2737 bc= -0.0001 cc= 38.8699 2 I(127) aa= -2968.5874 ba= -0.2318 ca= -39.1083 ab= -0.2318 bb= 1466.2555 cb= 0.0133 ac= -39.1083 bc= 0.0133 cc= 1502.3319
H_2S:ICl MP2= -1153.50435317 NIMAG= 0 Cl 3.116480000 -0.163547000 0.000328000 I 0.754724000 -0.118158000 -0.000354000 S -2.276249000 -0.044438000 -0.000945000 H -2.356993000 0.876641000 0.966520000 H -2.357471000 0.879597000 -0.965548000	1 Cl(35) aa= -74.6170 ba= -0.0066 ca= -1.5187 ab= -0.0066 bb= 37.2502 cb= 0.0001 ac= -1.5187 bc= 0.0001 cc= 37.3668 2 I(127) aa= -2895.9959 ba= -0.2919 ca= -51.4872 ab= -0.2919 bb= 1436.4053 cb= 0.0362 ac= -51.4872 bc= 0.0362 cc= 1459.5907
HC≡CH:ICl MP2= -831.75806105 NIMAG= 0 Cl 0.000000000 0.000000000 0.000000000 I 0.000000000 0.000000000 2.347643000 C 0.608205000 0.000000000 5.294826000 C -0.608205000 0.000000000 5.294826000 H 1.671450000 0.000000000 5.319881000 H -1.671450000 0.000000000 5.319881000	1 Cl(35) aa= -77.5842 ba= -0.0000 ca= -0.0000 ab= -0.0000 bb= 38.4475 cb= -0.0000 ac= -0.0000 bc= -0.0000 cc= 39.1367 2 I(127) aa= -2892.3823 ba= -0.0000 ca= -0.0000 ab= -0.0000 bb= 1376.7031 cb= -0.0000 ac= -0.0000 bc= -0.0000 cc= 1515.6792
$H_2C{=}CH_2$:ICl MP2= -833.00293154 NIMAG= 0 Cl 0.000000000 0.000000000 0.000000000 I 0.000000000 0.000000000 2.373496000 C 0.673443000 0.000000000 5.143060000 C -0.673443000 0.000000000 5.143060000 H 1.232844000 0.924988000 5.161848000 H 1.232844000 -0.924988000 5.161848000 H -1.232844000 -0.924988000 5.161848000 H -1.232844000 0.924988000 5.161848000	1 Cl(35) aa= -71.1773 ba= -0.0000 ca= -0.0000 ab= -0.0000 bb= 35.1373 cb= 0.0000 ac= -0.0000 bc= 0.0000 cc= 36.0400 2 I(127) aa= -2839.0195 ba= -0.0000 ca= 0.0000 ab= -0.0000 bb= 1330.8168 cb= -0.0000 ac= 0.0000 bc= -0.0000 cc= 1508.2027

PH_3:ICl
MP2= -1097.26137326 NIMAG= 0

Cl	0.000000000	0.000000000	0.000000000
I	0.000000000	0.000000000	2.414626000
P	0.000000000	0.000000000	5.207034000
H	1.228027000	0.000000000	5.889852000
H	-0.614013000	1.063502000	5.889852000
H	-0.614013000	-1.063502000	5.889852000

1 Cl(35)
aa= -62.0391 ba= 0.0000 ca= 0.0000
ab= 0.0000 bb= 31.0195 cb= -0.0000
ac= 0.0000 bc= -0.0000 cc= 31.0195
2 I(127)
aa= -2784.4494 ba= -0.0000 ca= 0.0000
ab= -0.0000 bb= 1392.2247 cb= -0.0000
ac= 0.0000 bc= -0.0000 cc= 1392.2247

NH_3:ICl
MP2= -811.06578565 NIMAG= 0

Cl	0.000000000	0.000000000	0.000000000
I	0.000000000	0.000000000	2.389605000
N	0.000000000	0.000000000	4.930021000
H	0.946555000	0.000000000	5.291610000
H	-0.473278000	0.819741000	5.291610000
H	-0.473278000	-0.819741000	5.291610000

1 Cl(35)
aa= -66.0142 ba= -0.0000 ca= -0.0000
ab= -0.0000 bb= 33.0071 cb= 0.0000
ac= -0.0000 bc= 0.0000 cc= 33.0071
2 I(127)
aa= -2993.8184 ba= -0.0000 ca= -0.0000
ab= -0.0000 bb= 1496.9092 cb= 0.0000
ac= -0.0000 bc= 0.0000 cc= 1496.9092

$N(CH_3)_3$:ICl
MP2= -928.72425726 NIMAG= ?

N	0.000000000	0.000000000	0.000000000
C	1.391595000	0.000000000	-0.462350000
C	-0.695798000	-1.205157000	-0.462350000
C	-0.695798000	1.205157000	-0.462350000
H	1.429909000	0.000000000	-1.557119000
H	-0.714955000	-1.238338000	-1.557119000
H	-0.714955000	1.238338000	-1.557119000
H	1.894219000	-0.885679000	-0.079781000
H	1.894219000	0.885679000	-0.079781000
H	-1.714130000	-1.197602000	-0.079781000
H	-0.180089000	-2.083281000	-0.079781000
H	-0.180089000	2.083281000	-0.079781000
H	-1.714130000	1.197602000	-0.079781000
I	0.000000000	0.000000000	2.392203000
Cl	0.000000000	0.000000000	4.829716000

14 I(127)
aa= -2844.6178 ba= 0.0000 ca= 0.0000
ab= 0.0000 bb= 1422.3089 cb= 0.0000
ac= 0.0000 bc= 0.0000 cc= 1422.3089
15 Cl(35)
aa= -58.1028 ba= 0.0000 ca= 0.0000
ab= 0.0000 bb= 29.0514 cb= 0.0000
ac= 0.0000 bc= 0.0000 cc= 29.0514

Table S5. Electronic energy (hartree) and optimized geometry (Å) at MP2/aug-cc-pVTZ computational level and Nuclear quadrupole coupling constants (MHz) at MP2/aug-cc-pV5Z level for B:IBr complexes.

Electronic energy (hartree) and optimized geometry (Å)				Nuclear quadrupole coupling constants (MHz)			
IBr				1 Br(79)			
MP2= -2867.57512959 NIMAG= 0				aa= 653.0369	ba= -0.0000	ca= -0.0000	
Br	0.000000000	0.000000000	0.000000000	ab= -0.0000	bb= -326.5184	cb= -0.0000	
I	0.000000000	0.000000000	2.465115000	ac= -0.0000	bc= -0.0000	cc= -326.5184	
				2 I(127)			
				aa= -2659.4859	ba= 0.0000	ca= 0.0000	
				ab= 0.0000	bb= 1329.7430	cb= 0.0000	
				ac= 0.0000	bc= 0.0000	cc= 1329.7430	
N_2:IBr				1 Br(79)			
MP2= -2976.94499087 NIMAG= 0				aa= 630.7291	ba= -0.0000	ca= -0.0000	
Br	0.000000000	0.000000000	0.000000000	ab= -0.0000	bb= -315.3646	cb= -0.0000	
I	0.000000000	0.000000000	2.469958000	ac= -0.0000	bc= -0.0000	cc= -315.3646	
N	0.000000000	0.000000000	5.548292000	2 I(127)			
N	0.000000000	0.000000000	6.662567000	aa= -2699.5099	ba= 0.0000	ca= 0.0000	
				ab= 0.0000	bb= 1349.7549	cb= 0.0000	
				ac= 0.0000	bc= 0.0000	cc= 1349.7549	
CO:IBr				1 Br(79)			
MP2= -2980.72494573 NIMAG= 0				aa= 601.6751	ba= -0.0000	ca= -0.0000	
Br	0.000000000	0.000000000	0.000000000	ab= -0.0000	bb= -300.8376	cb= -0.0000	
I	0.000000000	0.000000000	2.480117000	ac= -0.0000	bc= -0.0000	cc= -300.8376	
C	0.000000000	0.000000000	5.437837000	2 I(127)			
O	0.000000000	0.000000000	6.574862000	aa= -2733.3085	ba= 0.0000	ca= 0.0000	
				ab= 0.0000	bb= 1366.6542	cb= 0.0000	
				ac= 0.0000	bc= 0.0000	cc= 1366.6542	
HC≡N:IBr				1 Br(79)			
MP2= -2960.84704060 NIMAG= 0				aa= 579.0341	ba= -0.0000	ca= -0.0000	
Br	0.000000000	0.000000000	0.000000000	ab= -0.0000	bb= -289.5170	cb= -0.0000	
I	0.000000000	0.000000000	2.487337000	ac= -0.0000	bc= -0.0000	cc= -289.5170	
N	0.000000000	0.000000000	5.261124000	2 I(127)			
C	0.000000000	0.000000000	6.426268000	aa= -2804.0801	ba= 0.0000	ca= 0.0000	
H	0.000000000	0.000000000	7.492154000	ab= 0.0000	bb= 1402.0400	cb= 0.0000	
				ac= 0.0000	bc= 0.0000	cc= 1402.0400	
H_2O:IBr				1 Br(79)			
MP2= -2943.91496486 NIMAG= 0				aa= 591.1420	ba= -0.0000	ca= 6.0433	
Br	1.887967000	0.016522000	0.000000000	ab= -0.0000	bb= -294.9945	cb= 0.0000	
I	-0.596178000	-0.018254000	0.000000000	ac= 6.0433	bc= 0.0000	cc= -296.1475	
O	-3.376957000	-0.049374000	0.000000000	2 I(127)			
H	-3.764099000	0.393455000	0.762831000	aa= -2787.3997	ba= 0.0000	ca= -22.0146	
H	-3.764099000	0.393455000	-0.762831000	ab= 0.0000	bb= 1378.6448	cb= -0.0000	
				ac= -22.0146	bc= -0.0000	cc= 1408.7549	
H_2S:IBr				1 Br(79)			
MP2= -3266.49571655 NIMAG= 0				aa= 572.0996	ba= -0.0000	ca= 10.6749	
Br	-2.200748000	-0.025567000	0.000000000	ab= -0.0000	bb= -285.7261	cb= 0.0000	
I	0.300996000	0.029240000	0.000000000	ac= 10.6749	bc= 0.0000	cc= -286.3735	
S	3.387478000	0.067093000	0.000000000	2 I(127)			
H	3.481519000	-0.854482000	0.965551000	aa= -2729.6378	ba= -0.0000	ca= -43.8154	
H	3.481519000	-0.854482000	-0.965551000	ab= -0.0000	bb= 1355.0817	cb= 0.0000	
				ac= -43.8154	bc= 0.0000	cc= 1374.5562	
HC≡CH:IBr				1 Br(79)			
MP2= -2944.74979986 NIMAG= 0				aa= 593.5605	ba= -0.0000	ca= 0.0000	
Br	0.000000000	0.000000000	0.000000000	ab= -0.0000	bb= -294.8278	cb= 0.0000	
I	0.000000000	0.000000000	2.488548000	ac= 0.0000	bc= 0.0000	cc= -298.7326	
C	0.607942000	0.000000000	5.493094000	2 I(127)			
C	-0.607942000	0.000000000	5.493094000	aa= -2717.1576	ba= -0.0000	ca= -0.0000	
H	1.671142000	0.000000000	5.512059000	ab= -0.0000	bb= 1301.4062	cb= 0.0000	
H	-1.671142000	0.000000000	5.512059000	ac= -0.0000	bc= 0.0000	cc= 1415.7513	
$H_2C=CH_2$:IBr				1 Br(79)			
MP2= -2945.99414904 NIMAG= 0				aa= 552.1852	ba= -0.0000	ca= -0.0000	
Br	0.000000000	0.000000000	0.000000000	ab= -0.0000	bb= -273.7326	cb= 0.0000	
I	0.000000000	0.000000000	2.511556000	ac= -0.0000	bc= 0.0000	cc= -278.4526	
C	0.672390000	0.000000000	5.347376000	2 I(127)			
C	-0.672390000	0.000000000	5.347376000	aa= -2692.4888	ba= -0.0000	ca= -0.0000	
H	1.232246000	0.924886000	5.361530000	ab= -0.0000	bb= 1273.3789	cb= -0.0000	
H	1.232246000	-0.924886000	5.361530000	ac= -0.0000	bc= -0.0000	cc= 1419.1099	
H	-1.232246000	-0.924886000	5.361530000				
H	-1.232246000	0.924886000	5.361530000				

PH_3:IBr MP2= -3210.25168113 NIMAG= 0 Br 0.000000000 0.000000000 0.000000000 I 0.000000000 0.000000000 2.546933000 P 0.000000000 0.000000000 5.415252000 H 1.223263000 0.000000000 6.108610000 H -0.611631000 1.059377000 6.108610000 H -0.611631000 -1.059377000 6.108610000	1 Br(79) aa= 494.4916 ba= 0.0000 ca= 0.0000 ab= 0.0000 bb= -247.2458 cb= -0.0000 ac= 0.0000 bc= -0.0000 cc= -247.2458 2 I(127) aa= -2671.0814 ba= -0.0000 ca= -0.0000 ab= -0.0000 bb= 1335.5407 cb= -0.0000 ac= -0.0000 bc= -0.0000 cc= 1335.5407
NH_3:IBr MP2= -2924.05598844 NIMAG= 0 Br 0.000000000 0.000000000 0.000000000 I 0.000000000 0.000000000 2.529394000 N 0.000000000 0.000000000 5.111855000 H 0.946249000 0.000000000 5.474076000 H -0.473125000 0.819476000 5.474076000 H -0.473125000 -0.819476000 5.474076000	1 Br(79) aa= 507.2672 ba= 0.0000 ca= -0.0000 ab= 0.0000 bb= -253.6336 cb= 0.0000 ac= -0.0000 bc= 0.0000 cc= -253.6336 2 I(127) aa= -2846.8732 ba= -0.0000 ca= -0.0000 ab= -0.0000 bb= 1423.4366 cb= 0.0000 ac= -0.0000 bc= 0.0000 cc= 1423.4366
$N(CH_3)_3$:IBr MP2= -3041.71462521 NIMAG= ? N 0.000000000 0.000000000 0.000000000 C 1.391760000 0.000000000 -0.457956000 C -0.695880000 -1.205299000 -0.457956000 C -0.695880000 1.205299000 -0.457956000 H 1.434752000 0.000000000 -1.552872000 H -0.717376000 -1.242532000 -1.552872000 H -0.717376000 1.242532000 -1.552872000 H 1.893576000 -0.885708000 -0.074100000 H 1.893576000 0.885708000 -0.074100000 H -1.713834000 -1.197031000 -0.074100000 H -0.179742000 -2.082739000 -0.074100000 H -0.179742000 2.082739000 -0.074100000 H -1.713834000 1.197031000 -0.074100000 I 0.000000000 0.000000000 2.414720000 Br 0.000000000 0.000000000 4.995842000	14 I(127) aa= -2721.3614 ba= 0.0000 ca= 0.0000 ab= 0.0000 bb= 1360.6807 cb= 0.0000 ac= 0.0000 bc= 0.0000 cc= 1360.6807 15 Br(79) aa= 442.4027 ba= 0.0000 ca= 0.0000 ab= 0.0000 bb= -221.2014 cb= 0.0000 ac= 0.0000 bc= 0.0000 cc= -221.2014

Table S6. Electronic energy (hartree) and optimized geometry (Å) at MP2/aug-cc-pVTZ computational level and Nuclear quadrupole coupling constants (MHz) at MP2/aug-cc-pV5Z level for B:I_2 complexes.

Electronic energy (hartree) and optimized geometry (Å)	Nuclear quadrupole coupling constants (MHz)
I_2 MP2= -589.76803158 NIMAG= 0 I 0.000000000 0.000000000 0.000000000 I 0.000000000 0.000000000 2.662589000	1 I(127) aa= -2326.4611 ba= 0.0000 ca= 0.0000 ab= 0.0000 bb= 1163.2306 cb= 0.0000 ac= 0.0000 bc= 0.0000 cc= 1163.2306 2 I(127) aa= -2326.4611 ba= 0.0000 ca= 0.0000 ab= 0.0000 bb= 1163.2306 cb= 0.0000 ac= 0.0000 bc= 0.0000 cc= 1163.2306
N_2:I_2 MP2= -699.13717650 NIMAG= 0 I 0.000000000 0.000000000 0.000000000 I 0.000000000 0.000000000 2.667127000 N 0.000000000 0.000000000 5.835807000 N 0.000000000 0.000000000 6.950154000	1 I(127) aa= -2271.0214 ba= 0.0000 ca= 0.0000 ab= 0.0000 bb= 1135.5107 cb= 0.0000 ac= 0.0000 bc= 0.0000 cc= 1135.5107 2 I(127) aa= -2362.6144 ba= 0.0000 ca= 0.0000 ab= 0.0000 bb= 1181.3072 cb= 0.0000 ac= 0.0000 bc= 0.0000 cc= 1181.3072
CO:I_2 MP2= -702.91624462 NIMAG= 0 I 0.000000000 0.000000000 0.000000000 I 0.000000000 0.000000000 2.673119000 C 0.000000000 0.000000000 5.782888000 O 0.000000000 0.000000000 6.920456000	1 I(127) aa= -2206.2561 ba= 0.0000 ca= 0.0000 ab= 0.0000 bb= 1103.1281 cb= 0.0000 ac= 0.0000 bc= 0.0000 cc= 1103.1281 2 I(127) aa= -2388.9267 ba= 0.0000 ca= 0.0000 ab= 0.0000 bb= 1194.4634 cb= 0.0000 ac= 0.0000 bc= 0.0000 cc= 1194.4634
HC≡N:I_2 MP2= -683.03765494 NIMAG= 0 I 0.000000000 0.000000000 0.000000000 I 0.000000000 0.000000000 2.680141000 N 0.000000000 0.000000000 5.567768000 C 0.000000000 0.000000000 6.733673000 H 0.000000000 0.000000000 7.799530000	1 I(127) aa= -2123.7509 ba= 0.0000 ca= 0.0000 ab= 0.0000 bb= 1061.8754 cb= 0.0000 ac= 0.0000 bc= 0.0000 cc= 1061.8754 2 I(127) aa= -2462.7334 ba= 0.0000 ca= 0.0000 ab= 0.0000 bb= 1231.3667 cb= 0.0000 ac= 0.0000 bc= 0.0000 cc= 1231.3667
H_2O:I_2 MP2= -666.10586837 NIMAG= 0 I 1.708468000 0.010977000 0.000000000 I -0.969147000 -0.019172000 0.000000000 O -3.837513000 -0.042124000 0.000000000 H -4.241282000 0.385152000 0.762946000 H -4.241282000 0.385152000 -0.762946000	1 I(127) aa= -2146.5366 ba= 0.0000 ca= -17.7165 ab= 0.0000 bb= 1071.4283 cb= -0.0000 ac= -17.7165 bc= -0.0000 cc= 1075.1083 2 I(127) aa= -2448.1881 ba= 0.0000 ca= -15.0754 ab= 0.0000 bb= 1211.6282 cb= -0.0000 ac= -15.0754 bc= -0.0000 cc= 1236.5599
H_2S:I_2 MP2= -988.68642794 NIMAG= 0 I -2.006172000 -0.020443000 0.000000000 I 0.686053000 0.037795000 0.000000000 S 3.876089000 0.051764000 0.000000000 H 3.928203000 -0.873345000 0.964943000 H 3.928203000 -0.873345000 -0.964943000	1 I(127) aa= -2104.4790 ba= 0.0000 ca= -42.9475 ab= 0.0000 bb= 1051.6041 cb= -0.0000 ac= -42.9475 bc= -0.0000 cc= 1052.8749 2 I(127) aa= -2411.7570 ba= 0.0000 ca= -42.6497 ab= 0.0000 bb= 1199.0708 cb= -0.0000 ac= -42.6497 bc= -0.0000 cc= 1212.6862
HC≡CH:I_2 MP2= -666.94105229 NIMAG= 0 I 0.000000000 0.000000000 0.000000000 I 0.000000000 0.000000000 2.681663000 C 0.607569000 0.000000000 5.779930000 C -0.607569000 0.000000000 5.779930000 H 1.670568000 0.000000000 5.793812000 H -1.670568000 0.000000000 5.793812000	1 I(127) aa= -2164.2101 ba= 0.0000 ca= -0.0000 ab= 0.0000 bb= 1075.6768 cb= -0.0000 ac= -0.0000 bc= -0.0000 cc= 1088.5333 2 I(127) aa= -2389.5259 ba= 0.0000 ca= -0.0000 ab= 0.0000 bb= 1151.4525 cb= 0.0000 ac= -0.0000 bc= 0.0000 cc= 1238.0734
H_2C=CH_2:I_2 MP2= -668.18451767 NIMAG= 0 I 0.000000000 0.000000000 0.000000000 I 0.000000000 0.000000000 2.698756000 C 0.670827000 0.000000000 5.654224000 C -0.670827000 0.000000000 5.654224000 H 1.231339000 0.924648000 5.661941000 H 1.231339000 -0.924648000 5.661941000 H -1.231339000 -0.924648000 5.661941000 H -1.231339000 0.924648000 5.661941000	1 I(127) aa= -2063.4244 ba= 0.0000 ca= 0.0000 ab= 0.0000 bb= 1025.4410 cb= -0.0000 ac= 0.0000 bc= -0.0000 cc= 1037.9834 2 I(127) aa= -2392.0142 ba= 0.0000 ca= -0.0000 ab= 0.0000 bb= 1148.8964 cb= 0.0000 ac= -0.0000 bc= 0.0000 cc= 1243.1178

$PH_3:I_2$ MP2= -932.44090194 NIMAG= 0 I 0.000000000 0.000000000 0.000000000 I 0.000000000 0.000000000 2.720044000 P 0.000000000 0.000000000 5.752624000 H 1.213627000 0.000000000 6.466499000 H -0.606814000 1.051032000 6.466499000 H -0.606814000 -1.051032000 6.466499000	1 I(127) aa= -1945.0755 ba= -0.0000 ca= 0.0000 ab= -0.0000 bb= 972.5378 cb= 0.0000 ac= 0.0000 bc= 0.0000 cc= 972.5378 2 I(127) aa= -2412.4150 ba= 0.0000 ca= -0.0000 ab= 0.0000 bb= 1206.2075 cb= 0.0000 ac= -0.0000 bc= 0.0000 cc= 1206.2075
$NH_3:I_2$ MP2= -646.24471190 NIMAG= 0 I 0.000000000 0.000000000 0.000000000 I 0.000000000 0.000000000 2.716896000 N 0.000000000 0.000000000 5.388513000 H 0.945228000 0.000000000 5.753064000 H -0.472614000 0.818592000 5.753064000 H -0.472614000 -0.818592000 5.753064000	1 I(127) aa= -1895.5163 ba= 0.0000 ca= 0.0000 ab= 0.0000 bb= 947.7582 cb= -0.0000 ac= 0.0000 bc= -0.0000 cc= 947.7582 2 I(127) aa= -2540.9984 ba= -0.0000 ca= -0.0000 ab= -0.0000 bb= 1270.4992 cb= 0.0000 ac= -0.0000 bc= 0.0000 cc= 1270.4992
$N(CH_3)_3:I_2$ MP2= -763.90250007 NIMAG= ? N 0.000000000 0.000000000 0.000000000 C 1.391432000 0.000000000 -0.451276000 C -0.695716000 -1.205016000 -0.451276000 C -0.695716000 1.205016000 -0.451276000 H 1.442793000 0.000000000 -1.546556000 H -0.721396000 -1.249495000 -1.546556000 H -0.721396000 1.249495000 -1.546556000 H 1.892438000 -0.885646000 -0.065568000 H 1.892438000 0.885646000 -0.065568000 H -1.713211000 -1.196076000 -0.065568000 H -0.179227000 -2.081722000 -0.065568000 H -0.179227000 2.081722000 -0.065568000 H -1.713211000 1.196076000 -0.065568000 I 0.000000000 0.000000000 2.461057000 I 0.000000000 0.000000000 5.234430000	14 I(127) aa= -2486.5950 ba= 0.0000 ca= 0.0000 ab= 0.0000 bb= 1243.2975 cb= 0.0000 ac= 0.0000 bc= 0.0000 cc= 1243.2975 15 I(127) aa= -1648.2321 ba= 0.0000 ca= 0.0000 ab= 0.0000 bb= 824.1160 cb= 0.0000 ac= 0.0000 bc= 0.0000 cc= 824.1160

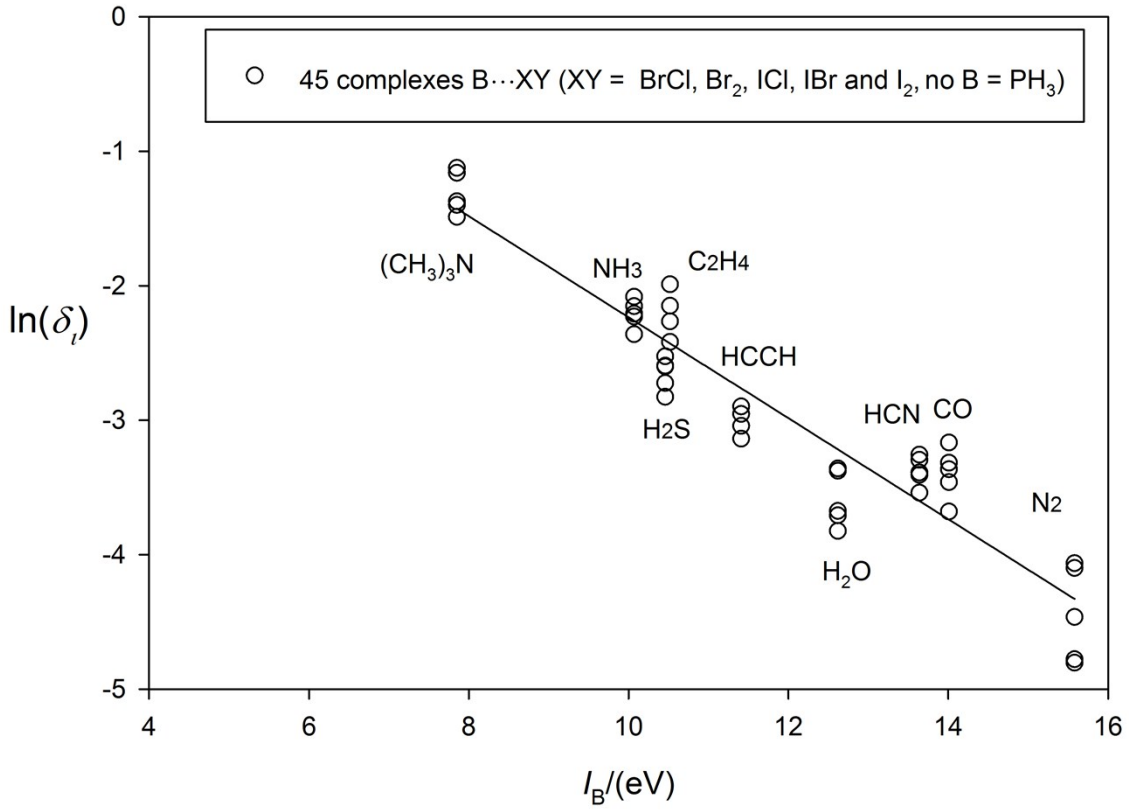

Figure S1. Plot of ln(δ_i) versus I_B for 18 complexes B···XY (B as indicated in the figure, X = Br or I, Y =Cl, Br or I). Note that the points for PH_3 are not included (see text). The solid line is the linear regression fit which is described by the equation ln(δ_i) =1.52(23)−0.376(20)(I_B/eV) and for which R^2 = 0.895.

Table S7. AIM charges (e) with the MP2/aug-cc-pVTZ wavefunction.

Base…Cl_2	Cl(inner)	Cl(outter)	sum	δ_i	δ_p
-	0.000	0.000	0.000		
Base= N_2	0.009	-0.012	-0.003	0.003	0.012
CO	0.009	-0.023	-0.013	0.013	0.023
HC≡N	0.029	-0.044	-0.015	0.015	0.044
H_2O	0.025	-0.042	-0.017	0.017	0.042
H_2S	-0.004	-0.046	-0.050	0.050	0.046
HC≡CH	0.002	-0.033	-0.031	0.031	0.033
$H_2C=CH_2$	-0.003	-0.048	-0.051	0.051	0.048
PH_3	-0.011	-0.059	-0.071	0.071	0.059
NH_3	0.025	-0.099	-0.074	0.074	0.099
$N(CH_3)_3$	-0.020	-0.295	-0.315	0.315	0.295

Base…BrCl	Br	Cl	sum	δ_i	δ_p
-	0.146	-0.146	0.000		
Base= N_2	0.161	-0.165	-0.004	0.004	0.018
CO	0.164	-0.185	-0.021	0.021	0.039
HC≡N	0.186	-0.209	-0.023	0.023	0.063
H_2O	0.178	-0.204	-0.026	0.026	0.058
H_2S	0.132	-0.218	-0.086	0.086	0.072
HC≡CH	0.148	-0.196	-0.048	0.048	0.050
$H_2C=CH_2$	0.139	-0.228	-0.089	0.089	0.081
PH_3	0.090	-0.313	-0.223	0.223	0.167
NH_3	0.169	-0.289	-0.121	0.121	0.143
$N(CH_3)_3$	0.134	-0.395	-0.261	0.261	0.249

Base…Br2	Br(inner)	Br(outter)	Sum	δ_i	δ_p
	0.000	0.000	0.000		
Base= N_2	0.016	-0.019	-0.003	0.003	0.019
CO	0.022	-0.038	-0.016	0.016	0.038
HC≡N	0.048	-0.067	-0.019	0.019	0.067
H_2O	0.040	-0.061	-0.021	0.021	0.061
H_2S	0.004	-0.078	-0.073	0.073	0.078
HC≡CH	0.012	-0.054	-0.041	0.041	0.054
$H_2C=CH_2$	0.012	-0.088	-0.076	0.076	0.088
PH_3	-0.006	-0.144	-0.150	0.150	0.144
NH_3	0.050	-0.154	-0.104	0.104	0.154
$N(CH_3)_3$	0.039	-0.294	-0.254	0.254	0.294

Base…ICl	I	Cl	Sum	δ_i	δ_p
-	0.327	-0.327	0.000		
Base= N_2	0.350	-0.351	-0.001	0.001	0.024
CO	0.363	-0.383	-0.020	0.020	0.056
HC≡N	0.383	-0.407	-0.024	0.024	0.080
H_2O	0.365	-0.393	-0.028	0.028	0.066
H_2S	0.310	-0.403	-0.093	0.093	0.076
HC≡CH	0.335	-0.386	-0.051	0.051	0.059
$H_2C=CH_2$	0.330	-0.421	-0.090	0.090	0.094
PH_3	0.290	-0.471	-0.182	0.182	0.144
NH_3	0.351	-0.465	-0.114	0.114	0.138
$N(CH_3)_3$	0.333	-0.512	-0.179	0.179	0.185

Base…IBr	I	Br	Sum	δ_i	δ_p
-	0.191	-0.191	0.000		
Base= N_2	0.216	-0.216	0.000	0.000	0.025
CO	0.231	-0.247	-0.016	0.016	0.056
HC≡N	0.257	-0.278	-0.020	0.020	0.086
H_2O	0.241	-0.264	-0.023	0.023	0.073
H_2S	0.195	-0.278	-0.083	0.083	0.087
HC≡CH	0.211	-0.256	-0.045	0.045	0.065
$H_2C=CH_2$	0.213	-0.295	-0.082	0.082	0.104
PH_3	0.190	-0.350	-0.160	0.160	0.159
NH_3	0.246	-0.352	-0.106	0.106	0.161
$N(CH_3)_3$	0.239	-0.417	-0.178	0.178	0.226

Base…I_2	I(inner)	I(outter)	Sum	δ_i	δ_p
-	0.000	0.000	0.000		
Base= N_2	0.026	-0.024	0.001	-0.001	0.024
CO	0.039	-0.050	-0.011	0.011	0.050
HC≡N	0.072	-0.086	-0.014	0.014	0.086
H_2O	0.060	-0.076	-0.016	0.016	0.076
H_2S	0.025	-0.091	-0.066	0.066	0.091
HC≡CH	0.031	-0.067	-0.035	0.035	0.067
$H_2C=CH_2$	0.040	-0.104	-0.064	0.064	0.104
PH_3	0.033	-0.147	-0.115	0.115	0.147
NH_3	0.085	-0.174	-0.088	0.088	0.174
$N(CH_3)_3$	0.100	-0.269	-0.168	0.168	0.269

Table S8. NBO charges (e) at the MP2/aug-cc-pVTZ computational level.

Base…Cl_2	Cl(inner)	Cl(outter)	Sum	δ_i	δ_p
-	0.000	0.000	0.000		
Base= N_2	0.006	-0.008	-0.002	0.002	0.008
CO	0.007	-0.018	-0.011	0.011	0.018
HC≡N	0.023	-0.032	-0.009	0.009	0.032
H_2O	0.016	-0.031	-0.015	0.015	0.031
H_2S	-0.007	-0.034	-0.041	0.041	0.034
HC≡CH	0.005	-0.020	-0.015	0.015	0.020
$H_2C=CH_2$	0.001	-0.032	-0.031	0.031	0.032
PH_3	-0.010	-0.045	-0.056	0.056	0.045
NH_3	0.009	-0.075	-0.066	0.066	0.075
$N(CH_3)_3$	-0.036	-0.256	-0.292	0.292	0.256

Base…BrCl	Br	Cl	Sum	δ_i	δ_p
-	0.106	-0.106	0.000		
Base= N_2	0.113	-0.119	-0.007	0.007	0.014
CO	0.109	-0.139	-0.030	0.030	0.033
HC≡N	0.132	-0.156	-0.024	0.024	0.050
H_2O	0.123	-0.153	-0.030	0.030	0.047
H_2S	0.076	-0.168	-0.092	0.092	0.062
HC≡CH	0.109	-0.143	-0.034	0.034	0.037
$H_2C=CH_2$	0.100	-0.172	-0.072	0.072	0.066
PH_3	0.015	-0.262	-0.247	0.247	0.156
NH_3	0.102	-0.232	-0.129	0.129	0.126
$N(CH_3)_3$	0.094	-0.341	-0.247	0.247	0.235
Base…Br_2	Br(inner)	Br(outter)	Sum	δ_i	δ_p
-	0.000	0.000			
Base= N_2	0.008	-0.013	-0.005	0.005	0.013
CO	0.007	-0.030	-0.023	0.023	0.030
HC≡N	0.031	-0.050	-0.019	0.019	0.050
H_2O	0.022	-0.047	-0.025	0.025	0.047
H_2S	-0.017	-0.060	-0.077	0.077	0.060
HC≡CH	0.007	-0.036	-0.029	0.029	0.036
$H_2C=CH_2$	0.002	-0.063	-0.062	0.062	0.063
PH_3	-0.044	-0.116	-0.160	0.160	0.116
NH_3	0.014	-0.124	-0.110	0.110	0.124
$N(CH_3)_3$	0.013	-0.254	-0.240	0.240	0.254

Base…ICl	I	Cl	Sum	δ_i	δ_p
	0.239	-0.239	0.000		
Base= N_2	0.249	-0.260	-0.011	0.011	0.021
CO	0.241	-0.296	-0.054	0.054	0.056
HC≡N	0.271	-0.312	-0.041	0.041	0.073
H_2O	0.257	-0.300	-0.043	0.043	0.061
H_2S	0.197	-0.315	-0.118	0.118	0.076
HC≡CH	0.246	-0.291	-0.045	0.045	0.051
$H_2C=CH_2$	0.244	-0.328	-0.085	0.085	0.089
PH_3	0.163	-0.391	-0.227	0.227	0.152
NH_3	0.235	-0.376	-0.141	0.141	0.137
$N(CH_3)_3$	0.244	-0.430	-0.186	0.186	0.191

Base…IBr	I	Br	Sum	δ_i	δ_p
-	0.137	-0.137	0.000		
Base= N_2	0.147	-0.157	-0.009	0.009	0.020
CO	0.144	-0.186	-0.042	0.042	0.049
HC≡N	0.175	-0.208	-0.034	0.034	0.071
H_2O	0.162	-0.199	-0.037	0.037	0.062
H_2S	0.108	-0.213	-0.105	0.105	0.076
HC≡CH	0.147	-0.187	-0.040	0.040	0.050
$H_2C=CH_2$	0.146	-0.224	-0.078	0.078	0.087
PH_3	0.086	-0.284	-0.198	0.198	0.147
NH_3	0.150	-0.281	-0.131	0.131	0.145
$N(CH_3)_3$	0.164	-0.349	-0.185	0.185	0.212

Base…I_2	I(inner)	I(outter)	Sum	δ_i	δ_p
-	0.000	0.000	0.000		
Base= N_2	0.012	-0.019	-0.007	0.007	0.019
CO	0.013	-0.041	-0.028	0.028	0.041
HC≡N	0.044	-0.067	-0.023	0.023	0.067
H_2O	0.033	-0.060	-0.027	0.027	0.060
H_2S	-0.010	-0.072	-0.081	0.081	0.072
HC≡CH	0.016	-0.047	-0.031	0.031	0.047
$H_2C=CH_2$	0.017	-0.078	-0.061	0.061	0.078
PH_3	-0.016	-0.120	-0.136	0.136	0.120
NH_3	0.035	-0.143	-0.107	0.107	0.143
$N(CH_3)_3$	0.054	-0.229	-0.175	0.175	0.229

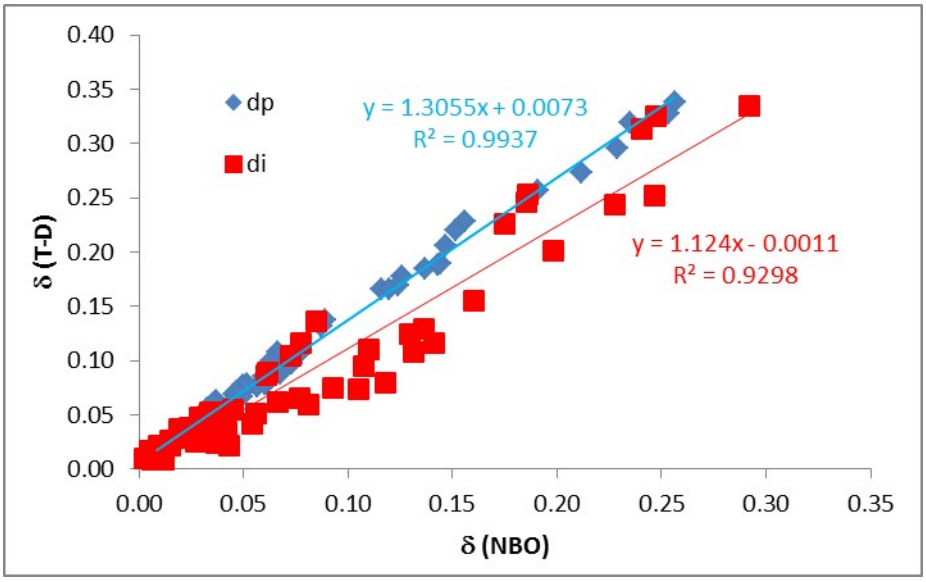

Figure S2. δ_i/δ_p values derived from the Townes-Dailey vs δ_i/δ_p (NBO).