Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

The Intrinsic Strength of the Halogen Bond: Electrostatic and Covalent Contributions

SUPPORTING INFORMATION

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Table S1: Summary of halogen acceptors properties

Acceptors	IP	NBO(A)	$V(\mathbf{r})_{min}$	α_{iso}	Dipole
NR_3					
NF_3	13.54	0.552	−2.20	18.6	0.242
NH_3	10.91	−1.022	−37.28	14.1	1.520
NHF_2	12.39	0.147	−16.08	16.5	1.920
NH_2F	11.60	−0.367	−27.87	14.9	2.269
NH_2CH_3	9.76	−0.813	−36.63	25.5	1.360
NH_2OH	10.75	−0.513	−26.46	18.8	0.601
NH_2CN	10.99	−0.821	−11.75	26.7	4.368
NH_2Cl	10.48	−0.751	−27.09	26.8	1.916
PR_3					
PF_3	12.28	1.717	2.55	25.8	1.153
PH_3	10.52	0.108	−15.68	30.2	0.606
PHF_2	10.94	1.324	−6.02	26.9	1.443
PH_2F	10.65	0.793	−11.16	28.4	1.428
PH_2CH_3	9.55	0.358	−21.04	42.3	1.139
PH_2OH	10.06	0.675	−14.55	33.3	0.688
PH_2CN	11.13	0.391	−1.34	42.4	3.551
PH_2Cl	10.20	0.413	−8.54	42.4	1.561
AR_2					
OH_2	12.43	−0.895	−32.34	9.5	1.845
SH_2	10.38	−0.232	−16.45	24.3	0.979
Anions					
F^-	3.31	−1.000	−168.62	8.8	0.000
Cl^-	3.51	−1.000	−139.48	28.1	0.000
Br^-	3.38	−1.000	−131.59	40.6	0.000

[a]. Computed at CCSD(T)/aug-cc-pVTZ. Vertical ionization potential in e.V. NBO charges at the XB acceptor heteroatom A, minimum electrostatic potential computed on the 0.001 e/Bohr^3 electron density surface at the lone pair region of A (V_{min}) in kcal/mol, isotropic polarizability α_{iso} in Bohr^3 and total dipole moment in Debye.

Table S2: Summary of halogen donors properties

Donors	r(YX)	k^a(YX)	n(YX)	NBO(X)	$V(\mathbf{r})_{max}$	α_{zz}	α_{iso}	Dipole
F_2	1.418	4.700	1.000	0.000	16.48	12.2	8.1	0.000
FCl	1.646	4.326	0.954	0.340	40.38	22.8	18.1	0.934
Cl_2	2.019	3.025	0.780	0.000	25.39	42.2	30.6	0.000
Br_2	2.313	2.340	0.675	0.000	28.50	62.6	45.0	0.000
O_2NCl	1.864	1.403	0.506	0.011	21.89	51.4	37.9	0.536
HCCCl	1.649	5.227	1.062	0.149	34.23	55.6	36.6	0.454
NCCl	1.644	5.209	1.060	0.171	36.76	45.3	30.4	2.865
H_2FP	1.577	5.791	1.125	0.793	36.57	28.7	28.4	1.428
HFS	1.626	4.569	0.984	0.406	40.28	22.7	23.8	1.491
FH	0.921	9.594	1.496	0.532	68.26	6.4	5.4	1.797

[a]. Computed at CCSD(T)/aug-cc-pVTZ. Bond distances r(YX) in Å, local YX stretching force constant $k^a(YX)$ in mdyn/Å, bond strength order n. NBO charges at X, maximum electrostatic potential computed on the 0.001 e/Bohr^3 electron density surface at the σ-hole of X (V_{max}) in kcal/mol, polarizability at the z direction α_{zz} and isotropic polarizability α_{iso} in Bohr^3 total dipole moment in Debye.

Table S3: Geometric and vibrational shifts of the YX bond for complexes 1 - 44.[a]

#	Complexes	ΔR(YX)	$\Delta\omega^a$(YX)	Δk^a(YX)	Δn(YX)
Dihalogens FCl		Å	cm^{-1}	mdyn/Å	
1	$F_2\cdots OH_2$ (C_s)	0.005	−21	−0.212	−0.026
2	$F_2\cdots NH_3$ (C_{3v})	0.014	−90	−0.879	−0.110
3	$F_2\cdots SH_2$ (C_s)	0.007	−46	−0.462	−0.057
4	$Cl_2\cdots OH_2$ (C_s)	0.008	−12	−0.129	−0.019
5	$Cl_2\cdots NH_3$ (C_{3v})	0.028	−62	−0.655	−0.100
6	$Cl_2\cdots SH_2$ (C_s)	0.013	−29	−0.310	−0.046
7	$Cl_2\cdots PH_3$ (C_{3v})	0.015	−38	−0.413	−0.062
Interhalogen FCl					
8	$FCl\cdots NF_3$ (C_{3v})	0.004	−9	−0.106	−0.013
9	$FCl\cdots NHF_2$ (C_s)	0.014	−42	−0.461	−0.058
10	$FCl\cdots NH_2F$ (C_s)	0.034	−112	−1.170	−0.155
11	$FCl\cdots NH_3$ (C_{3v})	0.057	−163	−1.639	−0.225
12	$FCl\cdots NH_2CN$ (C_s)	0.016	−52	−0.567	−0.072
13	$FCl\cdots NH_2Cl$ (C_s)	0.039	−124	−1.284	−0.172
14	$FCl\cdots NH_2OH$ (C_s) *syn*	0.066	−188	−1.854	−0.258
	$FCl\cdots NH_2OH$ (C_s) *anti*	0.054	−162	−1.629	−0.223
15	$FCl\cdots NH_2CH_3$ (C_s)	0.090	−216	−2.087	−0.296
16	$FCl\cdots OH_2$ (C_s)	0.014	−32	−0.359	−0.045
17	$FCl\cdots PF_3$ (C_{3v})	0.013	−72	−0.774	−0.100
18	$FCl\cdots PHF_2$ (C_s)	0.241	−364	−3.117	−0.489
19	$FCl\cdots PH_2F$ (C_s)	0.237	−383	−3.229	−0.514
20	$FCl\cdots PH_3$ (C_{3v})	0.139	−472	−3.672	−0.625
21	$FCl\cdots PH_2CN$ (C_s)	0.024	−144	−1.469	−0.199
22	$FCl\cdots PH_2Cl$ (C_s)	0.194	−397	−3.304	−0.531
23	$FCl\cdots PH_2OH$ (C_s) *syn*	0.270	−383	−3.231	−0.514
	$FCl\cdots PH_2OH$ (C_s) *anti*	0.258	−387	−3.253	−0.519
24	$FCl\cdots PH_2CH_3$ (C_s)	0.256	−394	−3.287	−0.527
25	$FCl\cdots SH_2$ (C_s)	0.027	−104	−1.089	−0.144
NH_3 Acceptor					
26	$HCCCl\cdots NH_3$ (C_{3v})	0.003	−14	−0.155	−0.018
27	$NCCl\cdots NH_3$ (C_{3v})	0.004	−23	−0.233	−0.027
28	$O_2NCl\cdots NH_3$ (C_s)	−0.025	32	0.189	0.037
29	$FH_2P\cdots NH_3$ (C_s)	0.067	−174	−1.997	−0.239
30	$FHS\cdots NH_3$ (C_s)	0.044	−120	−1.260	−0.164
31	$FH\cdots NH_3$ (C_{3v})	0.032	−772	−3.254	−0.312
Ionic Systems					
32	$[F\cdots F\cdots F]^-$ ($D_{\infty h}$)	0.321	−420	−3.324	−0.500
33	$[Cl\cdots Cl\cdots Cl]^-$ ($D_{\infty h}$)	0.309	−281	−2.324	−0.438
34	$[Br\cdots Br\cdots Br]^-$ ($D_{\infty h}$)	0.281	−140	−1.610	−0.325
35	$[F\cdots Cl\cdots F]^-$ ($D_{\infty h}$)	0.229	−319	−2.840	−0.432
36	$[F\cdots H\cdots F]^-$ ($D_{\infty h}$)	0.219	−2899	−8.746	−1.116
37	$[F\cdots PH_2\cdots F]^-$ (C_{2v})	0.259	−606	−4.534	−0.650
38	$FCl\cdots Cl^-$ ($C_{\infty v}$)	0.237	−363	−3.114	−0.489
39	$HCCCl\cdots Cl^-$ ($C_{\infty v}$)	0.008	−61	−0.628	−0.074
40	$NCCl\cdots Cl^-$ ($C_{\infty v}$)	0.015	−110	−1.083	−0.131
41	$O_2NCl\cdots Cl^-$ (C_{2v})	0.093	−136	−0.671	−0.156
42	$FH\cdots Cl^-$ ($C_{\infty v}$)	0.050	−1043	−4.239	−0.420
43	$FH_2P\cdots Cl^-$ (C_s)	0.148	−359	−3.655	−0.484
44	$FHS\cdots Cl^-$ (C_s)	0.164	−350	−3.103	−0.466

[a]. Shifts in the YX distances (ΔR), local mode stretching frequencies ($\Delta\omega^a$), local mode force constants (Δk^a) and bond strength order values (Δn) . Computed as the difference between the values in the monomer by the values in the complex. Calculated at CCSD(T)/aug-cc-pVTZ.

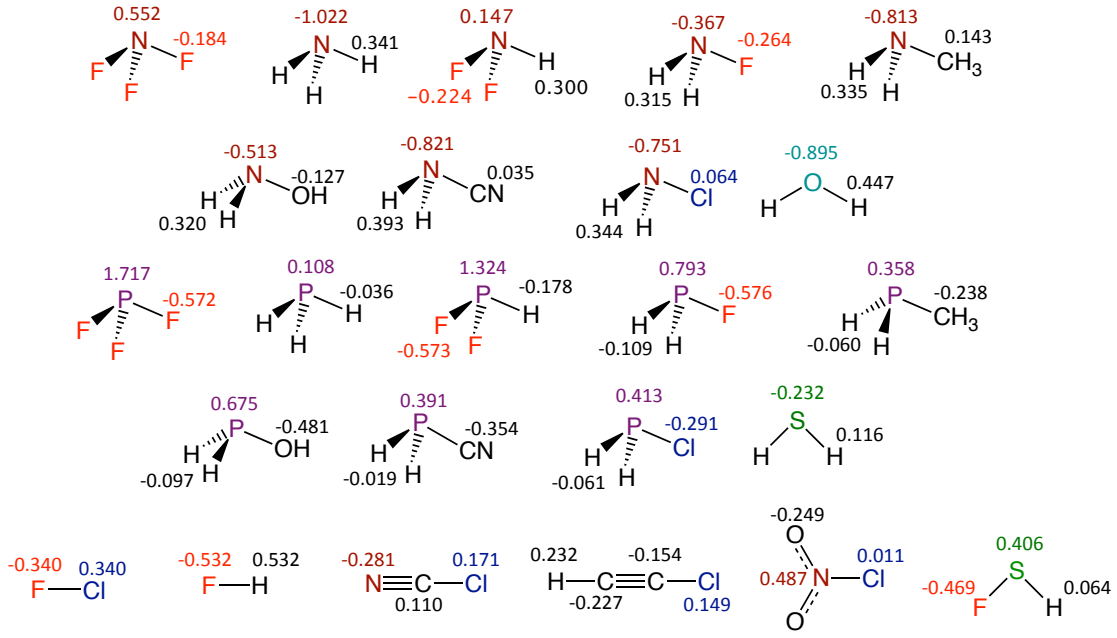


Figure S1: Schematic representation of the monomers with NBO atomic and group charges calculated at CCSD(T)/aug-cc-pVTZ.Color is used to relate charges to atoms.

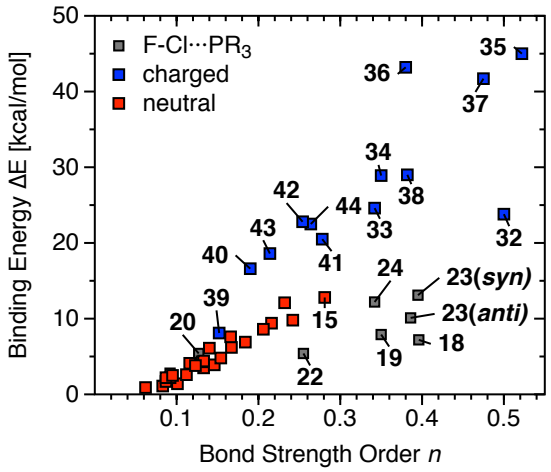


Figure S2: Comparison of the BSO n values and the binding energy of complexes.

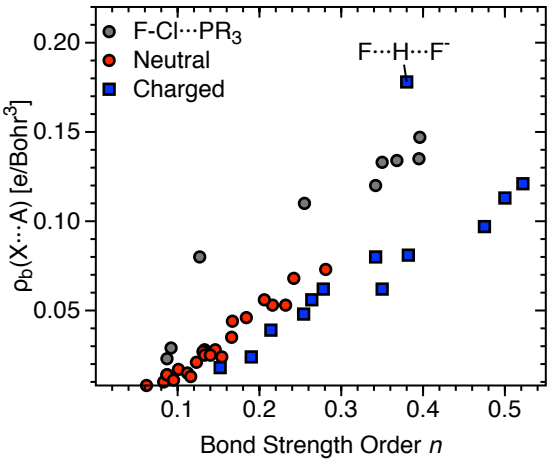
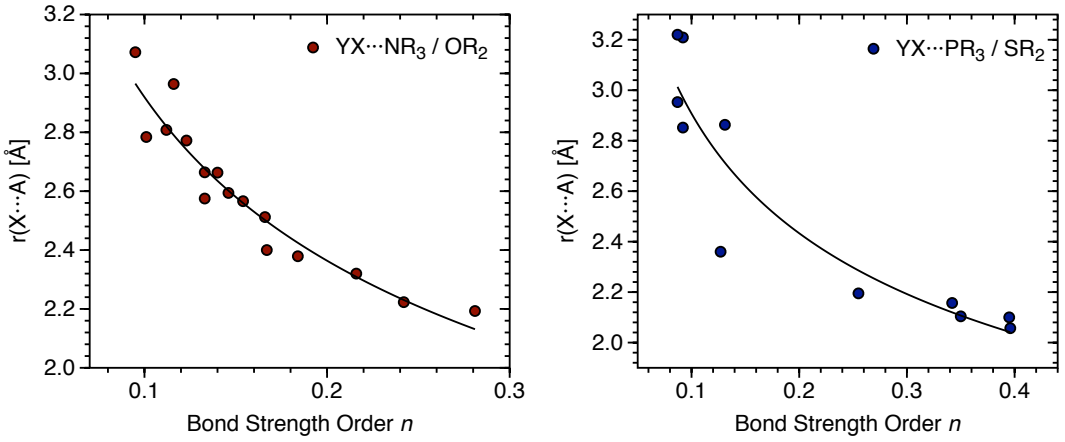


Figure S3: Comparison of the bond strength order (BSO) n with the density ρ_b at the critical point of the XB.



(a) (b)

Figure S4: Power relationship between the relative BSO n and the XB distance r(X$\cdots$A). a) Cl$\cdots$N and Cl$\cdots$O halogen bonding (R^2 is 0.919). b) Cl$\cdots$P and Cl$\cdots$S halogen bonding (R^2 is 0.879).

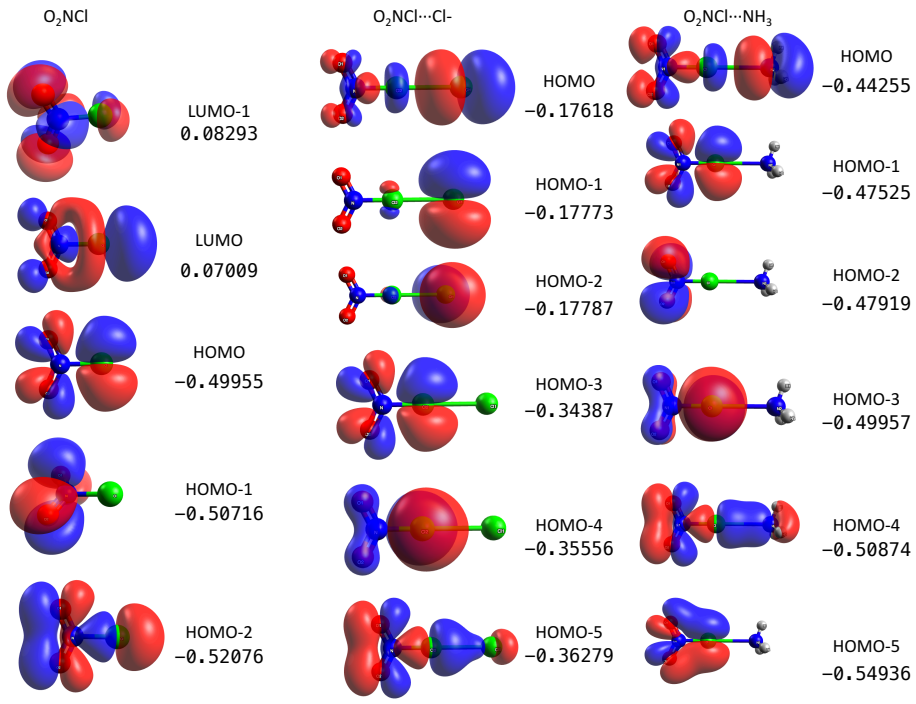


Figure S5: Obitals and orbital energies calculated at HF/6-31G(d) using an isosurface of 0.02 a.u. Orbital energies are given in Hartrees.

Table S4: Cartesian coordinates of dihalogen complexes 1-7

Atom type	x	y	z	Atom type	x	y	z
$F_2\cdots OH_2$				$Cl_2\cdots OH_2$			
E = -275.65824				E = -995.78482			
F	0.012431019	-0.386959569	0.000000000	CL	0.020320618	0.222572306	0.000000000
O	0.049559342	2.274274096	0.000000000	O	0.038496983	3.030078999	0.000000000
F	-0.012083069	-1.810089955	0.000000000	CL	-0.013654572	-1.804486643	0.000000000
H	-0.396550940	2.660984073	0.759300576	H	-0.421134587	3.399337359	0.760498875
H	-0.396550940	2.660984073	-0.759300576	H	-0.421134587	3.399337359	-0.760498875
$F_2\cdots NH_3$				$Cl_2\cdots NH_3$			
E = -255.79740				E = -975.92614			
F	-0.335737109	0.000000000	0.000000000	CL	-0.288680100	0.000000000	0.000000000
N	2.279248482	0.000000000	0.000000000	N	-2.952464092	0.000000000	0.000000000
F	-1.767928184	0.000000000	0.000000000	CL	1.758707678	0.000000000	0.000000000
H	2.662431813	-0.469847190	-0.813799204	H	-3.327827864	0.471348271	-0.816399153
H	2.662431813	0.939694380	0.000000000	H	-3.327827864	-0.942696541	0.000000000
H	2.662431813	-0.469847190	0.813799204	H	-3.327827864	0.471348271	0.816399153
$F_2\cdots SH_2$				$Cl_2\cdots SH_2$			
E = -598.25632				E = -1318.38273			
F	0.027665115	-2.506187326	0.000000000	CL	0.023419952	-2.397342513	0.000000000
F	-0.041774055	-1.082746594	0.000000000	CL	-0.037961192	-0.366402121	0.000000000
S	-0.047194112	2.008824605	0.000000000	S	-0.040172772	2.842481402	0.000000000
H	0.881572072	1.963501254	-0.967824381	H	0.889488335	2.860100981	-0.968390371
H	0.881572072	1.963501254	0.967824381	H	0.889488335	2.860100981	0.968390371
				$Cl_2\cdots PH_3$			
				-1262.13818			
				CL	0.390720978	0.000000000	0.000000000
				P	-2.828759508	0.000000000	0.000000000
				CL	2.424552488	0.000000000	0.000000000
				H	-3.581825246	0.600505569	-1.040106155
				H	-3.581825246	-1.201011138	0.000000000
				H	-3.581825246	0.600505569	1.040106155

[a]. Computed at CCSD(T)/aug-cc-pVTZ. the x, y, z coordinates are given in Å and the energy (E) is in Hartree.

Table S5: Cartesian coordinates of interhalogens complexes 8-25

Atom type	x	y	z	Atom type	x	y	z
$FCl\cdots NF_3$				$FCl\cdots PF_3$			
E = -913.11433				E = -1199.65894			
CL	-1.605537311	0.000000000	0.000000000	CL	-1.917672482	0.000000000	0.000000000
N	1.178762130	0.000000000	0.000000000	P	1.035643493	0.000000000	0.000000000
F	-3.255027320	0.000000000	0.000000000	F	-3.576552937	0.000000000	0.000000000
F	1.780462368	-0.615766106	-1.066538181	F	1.805938200	-0.685516106	-1.187348725
F	1.780462368	1.231532212	0.000000000	F	1.805938200	1.371032212	0.000000000
F	1.780462368	-0.615766106	1.066538181	F	1.805938200	-0.685516106	1.187348725
$FCl\cdots NF_2H$				$FCl\cdots PF_2H$			
E = -814.02484				E = -1100.46079			
F	-0.121602803	2.850622116	0.000000000	F	-0.132484382	2.986668450	0.000000000
CL	0.066020834	1.201645358	0.000000000	CL	0.034487887	1.107452088	0.000000000
N	0.398673184	-1.351780703	0.000000000	P	0.322822064	-0.929657857	0.000000000
F	-0.182204735	-1.985789128	1.093257362	F	-0.272430614	-1.717941555	1.205261861
F	-0.182204735	-1.985789128	-1.093257362	F	-0.272430614	-1.717941555	-1.205261861
H	1.331713534	-1.780763071	0.000000000	H	1.650553760	-1.386120086	0.000000000
$FCl\cdots NH_2F$				$FCl\cdots PH_2F$			
E = -714.94925				E = -1001.27356			
F	2.405489048	0.215395814	0.000000000	F	2.754681920	0.174085374	0.000000000
CL	0.756479467	-0.104065945	0.000000000	CL	0.879538232	0.004509532	0.000000000
N	-1.590479265	-0.604714240	0.000000000	P	-1.175986968	-0.445792215	0.000000000
H	-1.914735252	-1.117339444	0.820258354	H	-1.565619809	-1.232354105	1.096826378
H	-1.914735252	-1.117339444	-0.820258354	H	-1.565619809	-1.232354105	-1.096826378
F	-2.422447525	0.540409299	0.000000000	F	-2.290219768	0.675152494	0.000000000
$FCl\cdots NH_3$				$FCl\cdots PH_3$			
E = -615.89340				E = -902.10309			
CL	-0.115991624	0.000000000	0.000000000	CL	-1.917672558	0.000000000	0.000000000
N	2.204304739	0.000000000	0.000000000	P	1.035643491	0.000000000	0.000000000
F	-1.818970520	0.000000000	0.000000000	F	-3.576553029	0.000000000	0.000000000
H	2.562146782	-0.474369405	-0.821631910	F	1.805938279	-0.685516071	-1.187348665
H	2.562146782	0.948738809	0.000000000	F	1.805938279	1.371032143	0.000000000
H	2.562146782	-0.474369405	0.821631910	F	1.805938279	-0.685516071	1.187348665
$FCl\cdots NH_2CN$				$FCl\cdots PH_2CN$			
E = -707.96643				E = -994.19699			
F	2.689502623	0.409594032	0.000000000	F	3.154715194	0.485798853	0.000000000
CL	1.112457568	-0.115273934	0.000000000	CL	1.557848574	-0.003485958	0.000000000
N	-1.329708429	-0.990450550	0.000000000	P	-1.157966766	-0.872870893	0.000000000
H	-1.392077114	-1.562734999	0.834092679	H	-1.680819086	-1.659208507	1.052017087
H	-1.392077114	-1.562734999	-0.834092679	H	-1.680819086	-1.659208507	-1.052017087
C	-2.243485344	0.022104881	0.000000000	C	-2.468815383	0.352838747	0.000000000
N	-2.974336217	0.928609344	0.000000000	N	-3.251458496	1.216797937	0.000000000
$FCl\cdots NH_2Cl$				$FCl\cdots PH_2Cl$			
E = -1074.98320				E = -1361.26426			
F	2.815632122	0.365973791	0.000000000	F	3.154393896	0.380183087	0.000000000
CL	1.210104229	-0.143669755	0.000000000	CL	1.353408344	0.001608162	0.000000000
N	-1.048885033	-0.889989371	0.000000000	P	-0.724946777	-0.704148443	0.000000000
H	-1.259460888	-1.455539030	0.819374120	H	-1.004763115	-1.556475873	1.083485596
H	-1.259460888	-1.455539030	-0.819374120	H	-1.004763115	-1.556475873	-1.083485596
CL	-2.247206232	0.385128255	0.000000000	CL	-2.367135264	0.505259065	0.000000000
$FCl\cdots NH_2OH$				$FCl\cdots PH_2OH$			
E = -690.96669				E = -977.26803			
F	-2.249889834	0.275041397	0.000000000	F	-2.651344164	0.298884647	0.000000000
CL	-0.599385701	-0.180360963	0.000000000	CL	-0.790777251	-0.160158436	0.000000000
N	1.583429688	-0.601740954	0.000000000	P	1.286340656	-0.469503759	0.000000000
H	1.907519299	-1.097394366	0.826574146	H	1.838155568	-1.156544926	1.094675603
H	1.907519299	-1.097394366	-0.826574146	H	1.838155568	-1.156544926	-1.094675603
O	2.260056998	0.651943490	0.000000000	O	2.064917116	0.944207723	0.000000000
H	1.525018003	1.282042237	0.000000000	H	1.436576750	1.680044942	0.000000000
$FCl\cdots NH_2OH$ anti				$FCl\cdots PH_2OH$ anti			
E = -690.95766				E = -977.26286			
F	2.321531171	0.222162205	0.000000000	CL	-0.810506025	-0.088272463	0.000000000
CL	0.655259340	-0.113870503	0.000000000	P	1.256792684	-0.467829409	0.000000000
N	-1.595595437	-0.587217894	0.000000000	F	-2.683604559	0.254199466	0.000000000
H	-1.837536017	-1.122998384	0.830347690	H	1.727614172	-1.224001580	-1.091317918
H	-1.837536017	-1.122998384	-0.830347690	H	1.727614172	-1.224001580	1.091317918
O	-2.354414069	0.617769979	0.000000000	O	2.114407590	0.901582710	0.000000000
H	-3.287604375	0.363597864	0.000000000	H	3.072989093	0.788093113	0.000000000
$FCl\cdots NH_2CH_3$				$FCl\cdots PH_2CH_3$			
E = -655.12509				E = -941.36012			
F	-2.242284338	0.255703486	0.000000000	F	-2.664201959	0.314346217	0.000000000
CL	-0.553264166	-0.144799892	0.000000000	CL	-0.812985992	-0.119862072	0.000000000
N	1.592694131	-0.595193064	0.000000000	P	1.308886974	-0.506493433	0.000000000
H	1.789973574	-1.157695539	0.820596559	H	1.798642447	-1.253529851	1.086987619
H	1.789973574	-1.157695539	-0.820596559	H	1.798642447	-1.253529851	-1.086987619
C	2.363442396	0.657740943	0.000000000	C	2.286296400	1.030640931	0.000000000
H	2.085641859	1.233441272	0.882770797	H	2.013966413	1.605134003	0.886643041
H	2.085641859	1.233441272	-0.882770797	H	2.013966413	1.605134003	-0.886643041
H	3.444078039	0.490653097	0.000000000	H	3.356906843	0.824516019	0.000000000
$FCl\cdots OH_2$				$FCl\cdots SH_2$			
E = -635.74733				E = -958.34521			
CL	0.012719356	-0.213248144	0.000000000	CL	0.014033962	-0.747333287	0.000000000
O	0.048387159	2.352794232	0.000000000	S	0.050652484	2.115195165	0.000000000
F	-0.017869118	-1.873351478	0.000000000	F	-0.018555644	-2.420193658	0.000000000
H	-0.436209173	2.686471675	-0.762158165	H	-0.872020770	2.225601242	0.969476450
H	-0.436209173	2.686471675	0.762158165	H	-0.872020770	2.225601242	-0.969476450

[a]. Computed at CCSD(T)/aug-cc-pVTZ. the x, y, z coordinates are given in Å and the energy (E) is in Hartree.

Table S6: Cartesian coordinates of complexes 26-44

Atom type	x	y	z	Atom type	x	y	z
$HCCCl\cdots NH_3$				$HCCCl\cdots Cl^-$			
E = -592.80619				E = -996.13998			
H	3.865050892	0.000000000	0.000000000	H	0.000000000	0.000000000	4.433562461
C	2.802545657	0.000000000	0.000000000	C	0.000000000	0.000000000	3.372097421
C	1.591583919	0.000000000	0.000000000	C	0.000000000	0.000000000	2.156631216
CL	-0.060456119	0.000000000	0.000000000	CL	0.000000000	0.000000000	0.499964721
N	-3.132799693	0.000000000	0.000000000	CL	0.000000000	0.000000000	-2.524995381
H	-3.519771968	-0.469269718	-0.812798994				
H	-3.519771968	0.938539436	0.000000000				
H	-3.519771968	-0.469269718	0.812798994				
$NCCl\cdots NH_3$				$NCCl\cdots Cl^-$			
E = -608.89636				E = -1012.24109			
N	2.717308809	0.000000000	0.000000000	CL	0.000000000	0.000000000	2.452770130
C	1.551211363	0.000000000	0.000000000	CL	0.000000000	0.000000000	-0.430549126
CL	-0.096772635	0.000000000	0.000000000	C	0.000000000	0.000000000	-2.089937925
N	-3.060239003	0.000000000	0.000000000	N	0.000000000	0.000000000	-3.258962520
H	-3.449154070	-0.468993584	-0.812320716				
H	-3.449154070	0.937987168	0.000000000				
H	-3.449154070	-0.468993584	0.812320716				
$O2NCl\cdots NH_3$				$O_2NCl\cdots Cl^-$			
E = -721.03538				E = -1124.38726			
CL	-0.535291418	0.000823432	0.000000000	CL	0.000000000	0.000000000	-0.190171477
N	1.303400481	-0.000221123	0.000000000	N	0.000000000	0.000000000	1.766500350
O	1.810429243	-1.091838935	0.000000000	O	1.085973748	0.000000000	2.325893021
O	1.811722351	1.090791559	0.000000000	O	-1.085973748	0.000000000	2.325893021
N	-3.307699690	-0.000357522	0.000000000	CL	0.000000000	0.000000000	-2.644961735
H	-3.685462977	-0.942426034	0.000000000				
H	-3.689542582	0.469258828	-0.814776345				
H	-3.689542582	0.469258828	0.814776345				
$FH2P\cdots NH_3$				$FH2P\cdots Cl^-$			
E = -498.35328				E = -901.69817			
F	0.098328054	-1.858874375	0.000000000	P	0.694766491	0.154301664	0.000000000
P	-0.140894748	-0.232492435	0.000000000	F	2.399731174	-0.106610697	0.000000000
N	0.060446112	2.422509101	0.000000000	CL	-1.947202856	-0.033840356	0.000000000
H	0.958863624	2.895568050	0.000000000	H	0.486620909	-0.779158841	-1.040562036
H	-0.448021709	2.754819860	-0.813433699	H	0.486620909	-0.779158841	1.040562036
H	-0.448021709	2.754819860	0.813433699				
H	0.786952679	0.061150118	1.031500373				
H	0.786952679	0.061150118	-1.031500373				
$FHS\cdots NH_3$				$FHS\cdots Cl^-$			
E = -554.54106				E = -957.88982			
S	0.181284204	0.103332464	0.000000000	S	-0.613897362	0.124337004	0.000000000
F	1.841853155	-0.071197201	0.000000000	F	-2.391050996	-0.087111917	0.000000000
N	-2.326144458	-0.049210424	0.000000000	CL	1.873773647	-0.031757998	0.000000000
H	-0.052251468	-1.214434810	0.000000000	H	-0.466344720	-1.200390294	0.000000000
H	-2.613041047	0.924219792	0.000000000				
H	-2.743025126	-0.481004397	-0.818400169				
H	-2.743025126	-0.481004397	0.818400169				
$FH\cdots NH_3$				$FH\cdots Cl^-$			
E = -156.85044				E = -560.19270			
H	0.321576863	0.000000000	0.000000000	H	0.000000000	0.000000000	-0.882782706
N	-1.373847914	0.000000000	0.000000000	F	0.000000000	0.000000000	-1.853413993
F	1.274146369	0.000000000	0.000000000	CL	0.000000000	0.000000000	1.032392946
H	-1.750550445	0.471131031	-0.816022882				
H	-1.750550445	-0.942262061	0.000000000				
H	-1.750550445	0.471131031	0.816022882				
F_3^-				$FClF^-$			
E = -299.10106				E = -659.21983			
F	0.000000000	0.000000000	0.000000000	CL	0.000000000	0.000000000	0.000000000
F	0.000000000	0.000000000	-1.738658324	F	0.000000000	0.000000000	-1.875270215
F	0.000000000	0.000000000	1.738658324	F	0.000000000	0.000000000	1.875270215
Cl_3^-				Br_3^-			
E = -1379.28196				E = -7718.06495			
CL	0.000000000	0.000000000	0.000000000	BR	0.000000000	0.000000000	0.000000000
CL	0.000000000	0.000000000	-2.327707129	BR	0.000000000	0.000000000	-2.567163316
CL	0.000000000	0.000000000	2.327707129	BR	0.000000000	0.000000000	2.567163316
$FClF^-$				FHF^-			
E = -1019.24965				-200.17074			
CL	0.000000000	0.000000000	0.961107396	H	0.000000000	0.000000000	0.000000000
CL	0.000000000	0.000000000	-3.416315322	F	0.000000000	0.000000000	-1.140076297
F	0.000000000	0.000000000	4.519106337	F	0.000000000	0.000000000	1.140076297
$FH_2P\cdots F$-							
E = -541.68039							
P	0.000000000	0.000000000	-0.132137310				
F	1.825720435	0.000000000	0.065090586				
F	-1.825720435	0.000000000	0.065090586				
H	0.000000000	-1.063689437	0.803490248				
H	0.000000000	1.063689437	0.803490248				

[a]. Computed at CCSD(T)/aug-cc-pVTZ. the x, y, z coordinates are given in Å and the energy (E) is in Hartree.