Supporting Information

Using Beryllium Bonds to Change Halogen Bonds from Traditional to Chlorine-shared to Ion-Pair

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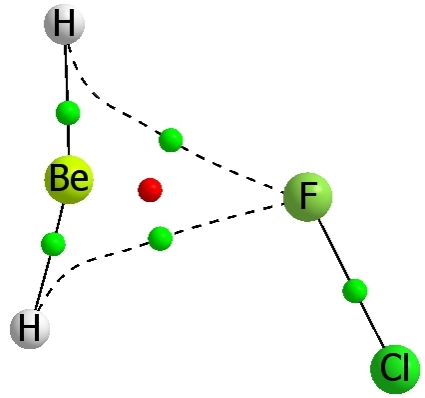
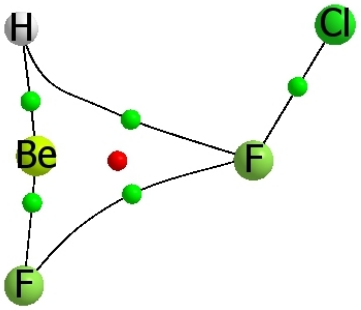
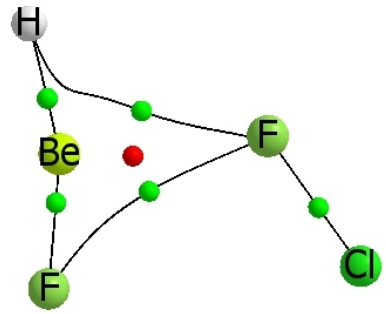
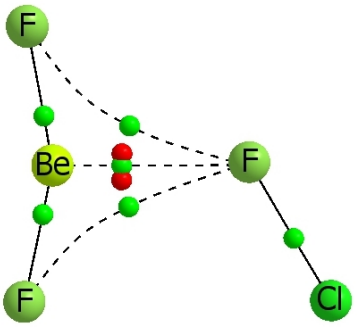
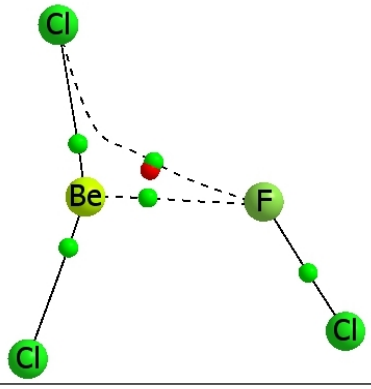
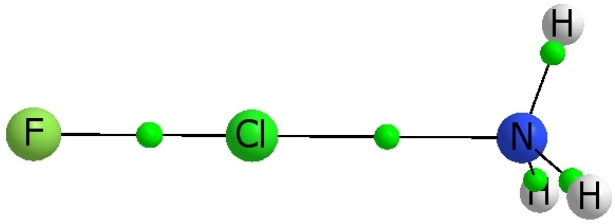
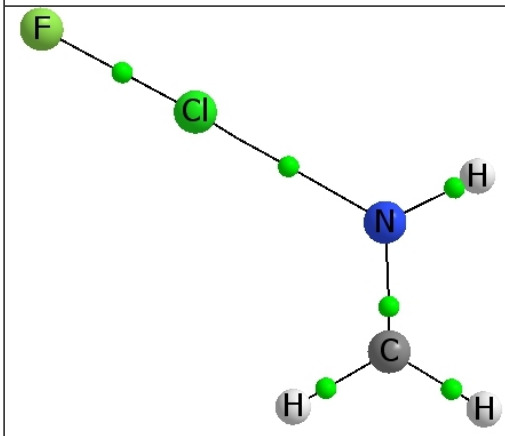
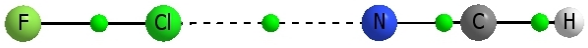
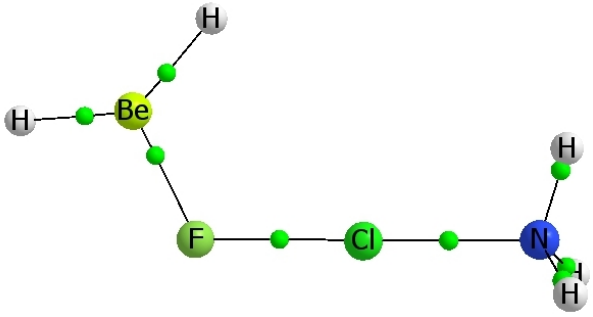
Table S1. MEP minima ($V_{S,Min}$) and maxima ($V_{S,Max}$) on the 0.001 au electron density isosurfaces of isolated monomers

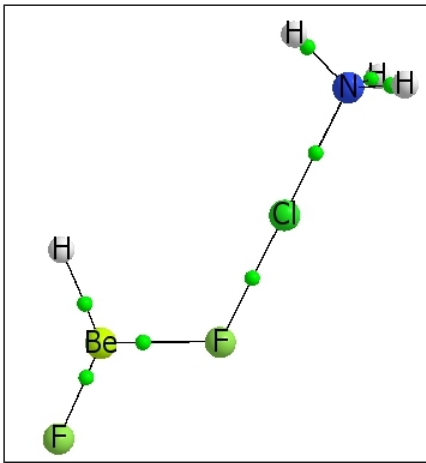
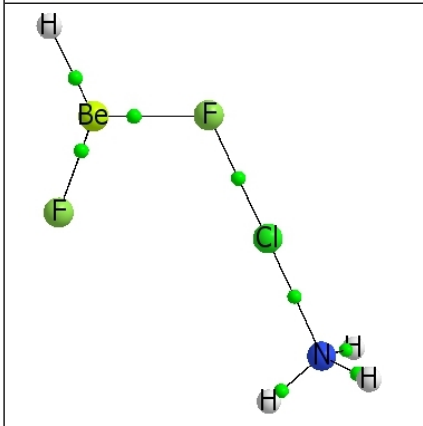
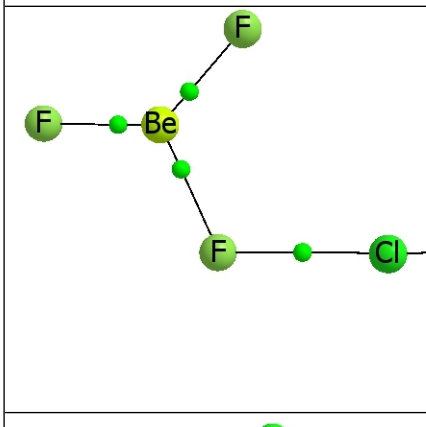
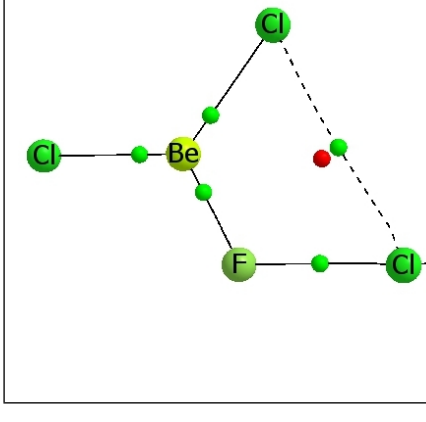
	$V_{S,Min}$ (au)	$V_{S,Max}$ (au)
BeH_2	–0.020	0.061
BeHF	–0.038 (F), –0.012 (H)	0.071
BeF_2	–0.034	0.103
$BeCl_2$	–0.008	0.061
FCl	–0.012	0.065

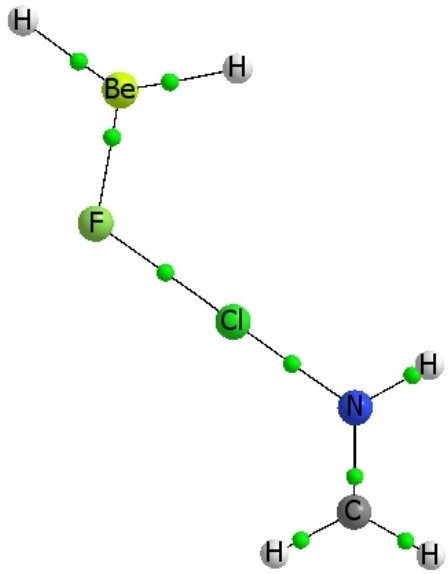
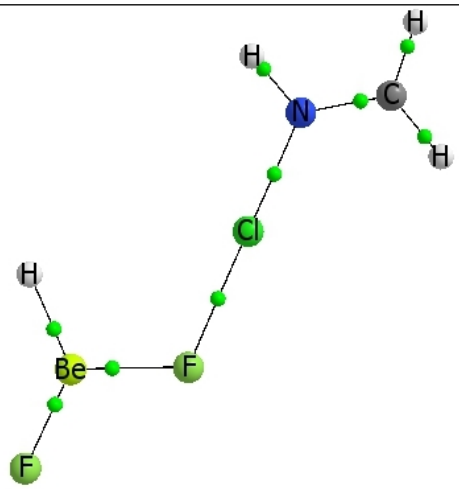
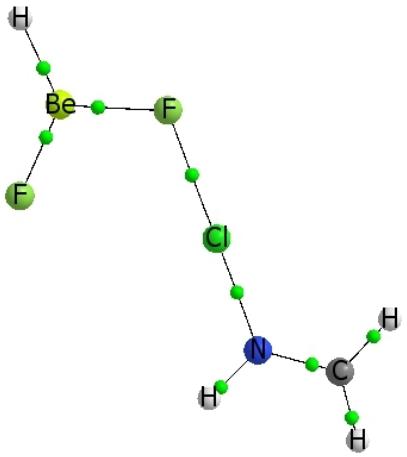
Nitrogen bases $V_{S,Min}$ (au)	
NH_3	–0.060
CH_2NH	–0.059
NCH	–0.066

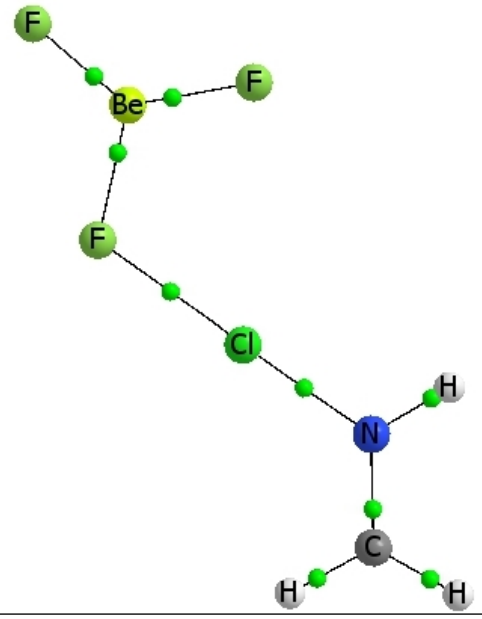
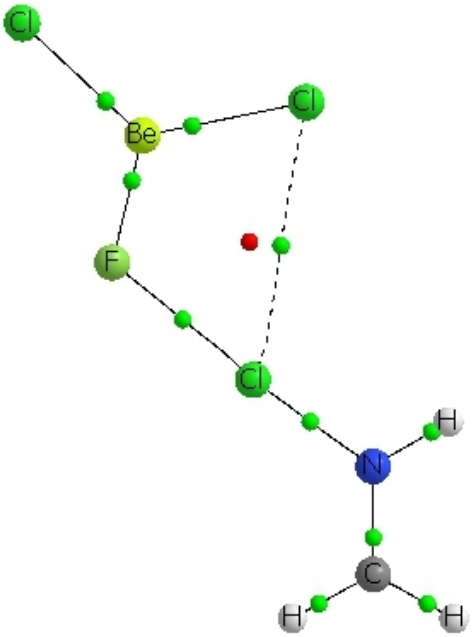
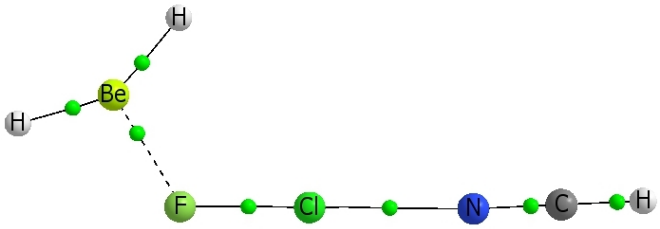
Table S2. MP2/aug'-cc-pVTZ total energies, geometries, and molecular graphs of binary complexes XYBe:FCl and FCl:N-base and ternary complexes XYBe:FCl:N-base

	beh2_fcl_augp MP2= -575.19788431 NIMAG= 0 Be,-3.2772199668,0.765823141,0. H,-2.539097152,1.8812736632,0. H,-4.2989938339,-0.0956730956,0. F,-1.7988585899,-0.670897137,0. Cl,-0.19701864,-0.2516192531,0.
	behf_fcl_E MP2= -674.45590581 NIMAG= 0 Be,-3.3462239451,0.8342679489,0. H,-2.5613247719,1.9078083697,0. F,-4.3803141623,-0.0885470989,0. F,-1.7004109947,-0.7522541148,0. Cl,-0.1229143085,-0.2723677864,0.
	behf_fcl_Z MP2= -674.45639874 NIMAG= 0 Be,-3.2965234122,0.7495937856,0. F,-2.5271975588,1.9106550705,0. H,-4.3305806783,-0.0894021576,0. F,-1.7758256736,-0.6933837213,0. Cl,-0.1810608598,-0.2485556587,0.
	bef2_fcl_augp MP2= -773.70622453 NIMAG= 0 Be,-3.2297578973,0.7191127181,0. F,-2.4926158771,1.9122685927,0. F,-4.3549159341,-0.1132219162,0. F,-1.8157929956,-0.6653948338,0. Cl,-0.2181054768,-0.2238572303,0.
	becl2_fcl_augp MP2= -1493.63195236 NIMAG= 0 Be,-3.1570054971,0.6732693946,0. Cl,-2.3388403304,2.3144543538,0. Cl,-4.653267555,-0.3831554272,0. F,-1.7969712432,-0.6536726164,0. Cl,-0.165103555,-0.3219883714,0.

	fcl_nh3_augp MP2= -615.83985723 NIMAG= 0 N X,1,1. H,1,r1,2,a1 H,1,r1,2,a1,3,120.,0 H,1,r1,2,a1,3,-120.,0 Cl,1,r2,3,a1,2,0.,0 F,1,r3,3,a1,2,0.,0 r1=1.01226254 a1=110.14516891 r2=2.23534533 r3=3.94891787
	fcl_nhch2_augp MP2= -653.82703879 NIMAG= 0 F,0.3052745941,0.,-0.9001821725 Cl,0.1734484303,0.,0.8157583439 N,-0.0621618853,0.,2.963727687 H,0.7252783156,0.,3.6095365324 C,-1.2092178271,0.,3.51550321 H,-2.0832423859,0.,2.8738250626 H,-1.3473022416,0.,4.5933303366
	fcl_nch_augp MP2= -652.63032400 NIMAG= 0 F,-0.2290622413,0.,0. Cl,1.4269806959,0.,0. N,3.968497268,0.,0. C,5.1335470031,0.,0. H,6.2000372742,0.,0.
	beh2_fcl_nh3_augp MP2= -631.70308400 NIMAG= 0 N,0.0440356751,0.,0.1479970865 H,1.0115155881,0.,-0.1632704846 H,-0.4312643848,-0.8332282283,-0.1854097209 H,-0.4312643848,0.8332282283,-0.1854097209 Cl,0.0580151058,0.,2.0621749946 F,0.105952045,0.,3.9795838915 Be,1.5641163168,0.,4.6554067024 H,2.5564066807,0.,3.6974930698 H,1.4980626454,0.,6.0186940143

	behf_fcl_nh3_E MP2= -730.96130536 NIMAG= 0 N,0.0420355342,0.,0.1401680661 H,1.0077226099,0.,-0.1771563173 H,-0.4351448248,-0.833269592,-0.1911945871 H,-0.4351448248,0.833269592,-0.1911945871 Cl,0.0617991658,0.,2.0453358801 F,0.0950224294,0.,3.9720370823 Be,1.5569634212,0.,4.6442240964 H,2.567736751,0.,3.7116142174 F,1.5145850255,0.,6.0734259833
	behf_fcl_nh3_Z MP2= -730.96323995 NIMAG= 0 N,0.0516217128,0.,0.1554504606 H,1.0245381812,0.,-0.1396134718 H,-0.4183468097,-0.8336362439,-0.1850464305 H,-0.4183468097,0.8336362439,-0.1850464305 Cl,0.0434161909,0.,2.0573778128 F,0.0686602715,0.,3.9954740317 Be,1.5267643525,0.,4.6604751966 F,2.5587092238,0.,3.6458276137 H,1.5385589728,0.,6.0223610495
	bef2_fcl_nh3_augp MP2= -830.21765989 NIMAG= 0 N,0.0557599013,0.,0.1609185011 H,1.0312892324,0.,-0.1275024084 H,-0.4115260313,-0.8337733438,-0.1844278916 H,-0.4115260313,0.8337733438,-0.1844278916 Cl,0.0315616282,0.,2.0423223184 F,0.053211555,0.,4.0004686943 Be,1.5128421655,0.,4.634388097 F,2.5507295019,0.,3.618361624 F,1.5632333678,0.,6.0671587858
	becl2_fcl_nh3_augp MP2= -1550.15347917 NIMAG= 0 N,0.0364724708,0.,0.1100791342 H,1.0214547824,0.,-0.1527265697 H,-0.421458306,-0.834969761,-0.2488562289 H,-0.421458306,0.834969761,-0.2488562289 Cl,-0.0248842127,0.,1.9406385898 F,0.0278707746,0.,3.9828492666 Be,1.4016211369,0.,4.6560930234 Cl,2.8989904798,0.,3.447233339 Cl,1.4569664566,0.,6.5408055126

	beh2_fcl_nhch2_augp MP2= -669.69539592 NIMAG= 0 F,0.347118782,0.,-1.0637328942 Cl,0.1566051033,0.,0.9176552329 N,0.0023583014,0.,2.6999131649 H,0.8869977375,0.,3.2049133227 C,-1.0983022427,0.,3.3404447014 H,-2.0200302237,0.,2.7744359316 H,-1.0932799972,0.,4.4224602192 Be,1.8371108053,0.,-1.5899559291 H,2.7429431363,0.,-0.537017805 H,1.9582805979,0.,-2.9545859444
	behf_fcl_nhch2_E MP2= -768.95399073 NIMAG= 0 F,0.3427480761,0.,-1.0556074225 Cl,0.1643764347,0.,0.9403897151 N,0.0002992471,0.,2.7145428144 H,0.8811830036,0.,3.2259810776 C,-1.1053416396,0.,3.3468308538 H,-2.0230939178,0.,2.7744669361 H,-1.1065660877,0.,4.42875921 Be,1.8307449084,0.,-1.584487254 H,2.7648309236,0.,-0.5629543613 F,1.9706210517,0.,-3.013391569
	behf_fcl_nhch2_Z MP2= -768.95588784 NIMAG= 0 F,0.3124735342,0.,-1.0948707727 Cl,0.1395621416,0.,0.9177576154 N,0.0022809055,0.,2.6888361304 H,0.8944109185,0.,3.1807387251 C,-1.090525737,0.,3.3431864808 H,-2.0196203851,0.,2.7896179431 H,-1.0689371645,0.,4.4248415545 Be,1.8039225818,0.,-1.600733156 F,2.737946154,0.,-0.4822610704 H,2.0082890511,0.,-2.9525834501

	bef2_fcl_nhch2 MP2= -868.21102416 NIMAG= 0 F,0.3017438496,0.,-1.1092199912 Cl,0.1219417755,0.,0.9256166036 N,-0.0021197029,0.,2.683307871 H,0.8948916929,0.,3.1666899407 C,-1.089783372,0.,3.3469749631 H,-2.0238502453,0.,2.8020878937 H,-1.0555042759,0.,4.4281042928 Be,1.7953520076,0.,-1.5789333528 F,2.7293227063,0.,-0.4547982888 F,2.0478088492,0.,-2.9953008517
	becl2_fcl_nhch2_augp MP2= -1588.14865291 NIMAG= 0 F,0.281876197,0.,-1.1266129652 Cl,0.0294211964,0.,0.9937622402 N,-0.0490913213,0.,2.7186909737 H,0.8678523899,0.,3.1657888417 C,-1.1144922168,0.,3.4193691885 H,-2.068012235,0.,2.9099612322 H,-1.0333048625,0.,4.497660169 Be,1.7067984504,0.,-1.6281925617 Cl,3.0625387492,0.,-0.2446127782 Cl,2.0362169375,0.,-3.4912852597
	beh2_fcl_nch_augp MP2= -668.47383432 NIMAG= 0 Be,-3.0198661065,0.6481860627,0. H,-2.3287696186,1.8104140651,0. H,-4.2257380205,0.0416959542,0. F,-1.8857660838,-0.6692173285,0. Cl,-0.1772276773,-0.3671785347,0. N,1.9628398326,0.0069859645,0. C,3.0939648988,0.2702211119,0. H,4.1339724351,0.5117115749,0.

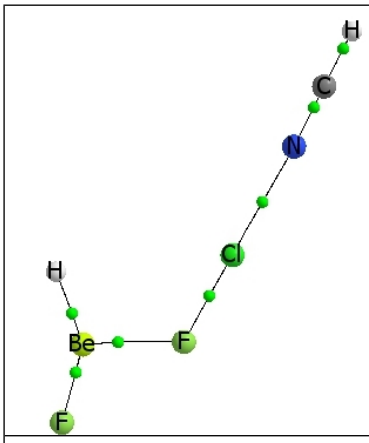
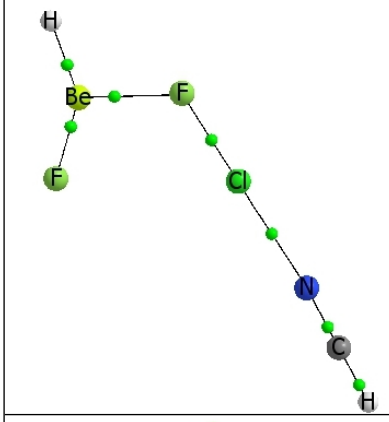
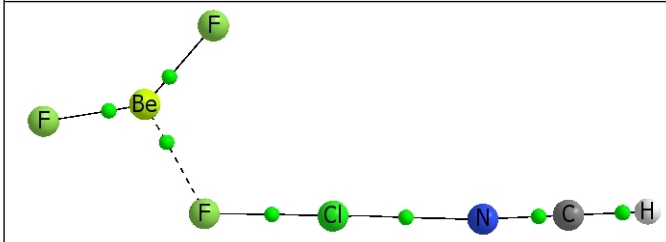
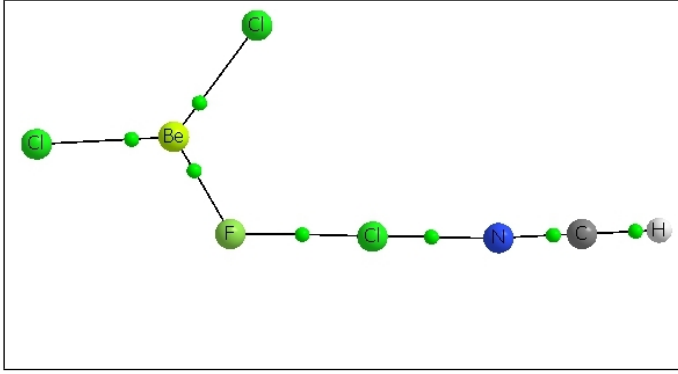
	behf_fcl_nch_E MP2= -767.73147105 NIMAG= 0 Be,-3.0044070757,0.6522275917,0. H,-2.3156447782,1.8115824443,0. F,-4.2817273801,0.0553154818,0. F,-1.8698948442,-0.697931699,0. Cl,-0.1670731176,-0.3770621595,0. N,1.9641557031,0.010215627,0. C,3.0943450931,0.2768827718,0. H,4.1336560593,0.5215888121,0.
	behf_fcl_nch_Z MP2= -767.73265806 NIMAG= 0 Be,-3.0049307077,0.6186179648,0. F,-2.2729819397,1.8313892626,0. H,-4.2390240976,0.0790473593,0. F,-1.88116488,-0.7018080059,0. Cl,-0.1639637565,-0.3903408646,0. N,1.9444818419,-0.0104681932,0. C,3.0684720082,0.280080368,0. H,4.1025211912,0.5463009789,0.
	bef2_fcl_nch_mp2_augp MP2= -866.98499789 NIMAG= 0 Be,-2.9437390724,0.5777827618,0. F,-2.2313849257,1.8130956642,0. F,-4.2657416036,0.0625316507,0. F,-1.8520155255,-0.719826109,0. Cl,-0.1140906941,-0.3796429497,0. N,1.895238388,0.0107699642,0. C,3.0161211676,0.3078008876,0. H,4.0490219258,0.580307,0.
	becl2_fcl_nch_mp2_augp MP2= -1586.91686046 NIMAG= 0 Be,-2.8351799681,0.426525859,0. Cl,-2.0379867977,2.1590412294,0. Cl,-4.6469178516,-0.0691714423,0. F,-1.8037461072,-0.7349608089,0. Cl,0.1221309612,-0.3605396779,0. N,1.8293826771,-0.0138567476,0. C,2.9459808993,0.2855853189,0. H,3.9797458468,0.5601951392,0.

Table S3. Electron density properties of FCl and binary and ternary complexes at bond critical points

F-Cl BCPs

Moiety	ρ_{bcp}	$\nabla^2\rho_{bcp}$	H_{bcp}
FCl	0.2120	–0.1845	–0.2152
H_2Be:FCl	0.2014	–0.1300	–0.1948
HFBe:FCl (E)	0.2052	–0.1499	–0.2029
HFBe:FCl (Z)	0.2013	–0.1299	–0.1950
F_2Be:FCl	0.1995	–0.1234	–0.1938
Cl_2Be:FCl	0.1953	–0.0998	–0.1843
FCl:NCH	0.2036	–0.1360	–0.1952
H2Be:FCl:NCH	0.1667	0.0466	–0.1225
HFBe:FCl:NCH (E)	0.1670	0.0444	–0.1241
HFBe:FCl:NCH (Z)	0.1623	0.0655	–0.1151
F_2Be:FCl:NCH	0.1523	0.1058	–0.0987
Cl_2Be:FCl:NCH	0.0948	0.2398	–0.0283
FCl:NH_3	0.1794	0.0093	–0.1381
H_2Be:FCl:NH_3	0.1082	0.2245	–0.0394
HFBe:FCl:NH_3 (E)	0.1053	0.2286	–0.0369
HFBe:FCl:NH_3 (Z)	0.1025	0.2308	–0.0341
F_2Be:FCl:NH_3	0.0972	0.2359	–0.0296
Cl_2Be:FCl:NH_3	0.0778	0.2395	–0.0152
FCl:$NHCH_2$	0.1767	0.0223	–0.1328
H_2Be:FCl:$NHCH_2$	0.0903	0.2400	–0.0239
HFBe:FCl:$NHCH_2$ (E)	0.0869	0.2413	–0.0214
HFBe:FCl:$NHCH_2$ (Z)	0.0836	0.2401	–0.0190
F_2Be:FCl:$NHCH_2$	0.0788	0.2395	–0.0157
Cl_2Be:FCl:$NHCH_2$	0.0619	0.2245	–0.0062

Cl···N BCPs

Moiety	ρ_{bcp}	$\nabla^2\rho_{bcp}$	H_{bcp}
FCl:NCH	0.0275	0.1098	0.0012
H_2Be:FCl:NCH	0.0657	0.1705	–0.0143
HFBe:FCl:NCH (E)	0.0666	0.1712	–0.0148
HFBe:FCl:NCH (Z)	0.0705	0.1730	–0.0171
F_2Be:FCl:NCH	0.0879	0.1752	–0.0288
Cl_2Be:FCl:NCH	0.1768	0.0064	–0.1352
FCl:NH_3	0.0646	0.1397	–0.0139
H_2Be:FCl:NH_3	0.1336	0.0696	–0.0670
HFBe:FCl:NH_3 (E)	0.1363	0.0632	–0.0698
HFBe:FCl:NH_3 (Z)	0.1373	0.0615	–0.0708
F_2Be:FCl:NH_3	0.1436	0.0455	–0.0777
Cl_2Be:FCl:NH_3	0.1607	–0.0037	–0.0976
FCl:$NHCH_2$	0.0750	0.1523	–0.0197
H_2Be:FCl:$NHCH_2$	0.1743	–0.0200	–0.1172
HFBe:FCl:$NHCH_2$ (E)	0.1773	–0.0312	–0.1214
HFBe:FCl:$NHCH_2$ (Z)	0.1793	–0.0376	–0.1244

F_2Be:FCl:$NHCH_2$	0.1852	–0.0612	–0.1335
Cl_2Be:FCl:$NHCH_2$	0.2009	–0.1280	–0.1583

Be···F BCPs[a]

Moiety	ρ_{bcp}	$\nabla^2\rho_{bcp}$	H_{bcp}
F_2Be:FCl	0.0214	0.0720	–0.0019
Cl_2Be:FCl	0.0260	0.1917	0.0048
H_2Be:FCl:NCH	0.0394	0.3857	0.0131
HFBe:FCl:NCH (E)	0.0376	0.3383	0.0104
HFBe:FCl:NCH (Z)	0.0411	0.3796	0.0114
H_2Be:FCl:NCH	0.0475	0.4300	0.0109
Cl_2Be:FCl:NCH	0.0783	0.7238	0.0072
H_2Be:FCl:NH_3	0.0633	0.6137	0.0128
HFBe:FCl:NH_3 (E)	0.0640	0.5994	0.0111
HFBe:FCl:NH_3 (Z)	0.0653	0.6151	0.0111
F_2Be:FCl:NH_3	0.0689	0.6333	0.0091
Cl_2Be:FCl:NH_3	0.0855	0.7866	0.0045
H_2Be:FCl:$NHCH_2$	0.0700	0.6732	0.0112
HFBe:FCl:$NHCH_2$ (E)	0.0712	0.6669	0.0096
HFBe:FCl:$NHCH_2$ (Z)	0.0723	0.6784	0.0095
F_2Be:FCl:$NHCH_2$	0.0755	0.6947	0.0075
Cl_2Be:FCl:$NHCH_2$	0.0916	0.8422	0.0020

Be···F BCPs (anions)

	ρ_{bcp}	$\nabla^2\rho_{bcp}$	H_{bcp}
BFH_2(–)	0.1002	0.9297	–0.0015
BF_2H(–)	0.1005	0.9268	–0.0022
BF_3(–)	0.1009	0.9221	–0.0030
$BFCl_2$(–)	0.1151	1.0549	–0.0103

a) No Be···F bond critical points are found for H_2Be:FCl and HFBe:FCl (E and Z). See molecular graphs in Table S1.

Table S4. NBO bond orders for FCl, binary complexes XYBe:FCl and FCl:N-base, and ternary complexes XYBe:FCl:N-base

Moiety	Be···F	F-Cl	Cl···N
FCl		0.5174	
H_2Be:FCl	0.1496	0.4801	
HFBe:FCl(E)	0.0714	0.4930	
HFBe:FCl (Z)	0.1072	0.4821	
F_2Be:FCl	0.1586	0.4861	
Cl_2Be:FCl	0.2334	0.4554	
FCl:NCH		0.4664	0.0968
H_2Be:FCl:NCH	0.2830	0.3815	0.2611
HFBe:FCl:NCH (E)	0.2419	0.3953	0.2658
HFBe:FCl:NCH (Z)	0.2596	0.3725	0.2763
F_2Be:FCl:NCH	0.3059	0.3331	0.3513
Cl_2Be:FCl:NCH	0.4287	0.1853	0.6933
FCl:NH_3		0.3766	0.2420
H_2Be:FCl:NH_3	0.3251	0.2220	0.4794
HFBe:FCl:NH_3 (E)	0.3256	0.2216	0.4902
HFBe:FCl:NH_3 (Z)	0.3348	0.2054	0.4808
F_2Be:FCl:NH_3	0.3769	0.1935	0.5312
Cl_2Be:FCl:NH_3	0.4540	0.1576	0.5916
FCl:$NHCH_2$		0.3698	0.2829
H_2Be:FCl:$NHCH_2$	0.3458	0.1774	0.6576
HFBe:FCl:$NHCH_2$ (E)	0.3477	0.1878	0.6688
HFBe:FCl:$NHCH_2$ (Z)	0.3539	0.1701	0.6694
F_2Be:FCl:$NHCH_2$	0.3976	0.1636	0.6896
Cl_2Be:FCl:$NHCH_2$	0.4766	0.1149	0.7473

Table S5. Many-body interaction energies (MBIE, kJ·mol^{-1}) in binary and ternary complexes

A:B	Er(A)	Er(B)	Δ^2E(A-B)	Ei (AB)
H_2Be:FCl	5.5	0.4	–15.4	–9.5
HFBe:FCl (E)	2.9	0.2	–11.6	–8.5
HFBe:FCl (Z)	6.3	0.4	–16.5	–9.8
F_2Be:FCl	11.1	0.5	–27.6	–16.0
Cl_2Be:FCl	17.7	1.0	–33.6	–14.9
B:C	Er(B)	Er(C)	Δ^2E(B-C)	Ei (BC)
FCl:NH_3	6.9	0.6	–56.5	–49.1
FCl:$NHCH_2$	8.2	2.1	–61.5	–51.2
FCl:NCH	0.4	0.0	–24.9	–24.5

A:B:C	ΔE	E_R(A)	E_R(B)	E_R(C)	Total E_R	Δ^2E(AB)	Δ^2E(AC)	Δ^2E(BC)	Total Δ^2E	Δ^3E(ABC)
H_2Be:FCl:NCH	–53.5	22.5	11.0	0.2	33.7	–32.4	–3.0	–21.6	–57	–30.1
HFBe:FCl:NCH (E)	–51.5	25.4	10.5	0.2	36.1	–30.5	–3.7	–20.9	–55.1	–32.5
HFBe:FCl:NCH (Z)	–54.6	27.5	13.1	0.2	40.8	–37.6	–3.4	–20.7	–61.7	–33.7
F_2Be:FCl:NCH	–67.5	38.1	19.3	0.3	57.7	–52.3	–5.1	–16.0	–73.4	–51.8
Cl_2Be:FCl:NCH	–82.4	65.2	83.7	0.7	149.6	–77.0	–6.6	–2.7	–86.3	–145.7
H_2Be:FCl:NH_3	–129.9	41.5	67.2	2.0	110.7	–51.1	–4.4	–84.3	–139.8	–100.7
HFBe:FCl:NH_3 (E)	–129.4	48.0	70.5	1.9	120.4	–43.7	–5.2	–85.0	–133.8	–116.0
HFBe:FCl:NH_3 (Z)	–134.5	50.7	74.7	2.0	127.4	–61.6	–5.6	–87.0	–154.1	–107.8
F_2Be:FCl:NH_3	–152.8	62.1	82.3	2.0	146.4	–68.1	–7.1	–88.0	–163.2	–136.0
Cl_2Be:FCl:NH_3	–178.2	75.1	114.8	2.2	192.1	–84.8	–7.4	–99.2	–191.4	–178.8
H_2Be:FCl:$NHCH_2$	–145.5	47.3	94.6	9.6	151.5	–57.0	–4.8	–107.9	–169.7	–127.4
HFBe:FCl:$NHCH_2$ (E)	–146.0	54.3	99.8	9.7	163.8	–45.3	–5.6	–109.9	–160.9	–148.9

HFBe:FCl:$NHCH_2$ (Z)	–151.0	57.8	106.0	9.9	173.7	–69.8	–6.1	–112.7	–188.5	–136.2
F_2Be:FCl:$NHCH_2$	–171.2	69.7	114.8	10.3	194.8	–70.7	–7.7	–115.3	–193.7	–172.2
Cl_2Be:FCl:$NHCH_2$	–201.3	82.0	149.8	11.4	243.2	–90.8	–8.2	–126.5	–225.5	–219.0

Table S6. Coupling constants (J) and their components (Hz) across Be···F, F-Cl, and Cl···N bonds

Moiety	PSO	DSO	FC	SD	^{1be}J(Be-F)
H_2Be:FCl	1.1	–0.2	22.2	–0.2	22.9
H_2Be:FCl:NH_3	4.3	–0.2	12.6	–0.2	16.5
H_2Be:FCl:$NHCH_2$	4.7	–0.2	4.6	–0.1	8.9
H_2Be:FCl:NCH	2.7	–0.2	36.7	–0.2	39.0
H_2BeF^-	6.8	0.0	–28.3	0.2	–21.4
HFBe:FCl (*E*)	0.6	–0.3	12.5	–0.2	12.6
HFBe:FCl:NH_3	3.4	–0.4	–1.8	–0.3	1.0
HFBe:FCl:$NHCH_2$	3.8	–0.3	–9.2	–0.2	–5.9
HFBe:FCl:NCH	2.0	–0.4	23.6	–0.4	24.9
$HBeF_2^-$	5.6	–0.2	–37.4	0.0	–32.0
HFBe:FCl (*Z*)	0.9	–0.3	25.7	–0.1	26.1
HFBe:FCl:NH_3	3.4	–0.3	4.4	–0.2	7.3
HFBe:FCl:$NHCH_2$	3.8	–0.3	–4.8	–0.2	–1.5
HFBe:FCl:NCH	2.1	–0.4	33.4	–0.2	34.9
$HBeF_2^-$	5.6	–0.2	–37.4	0.0	–32.0
F_2Be:FCl	1.0	–0.4	8.7	–0.2	9.0
F_2Be:FCl:NH_3	2.9	–0.5	–29.8	–0.3	–27.7
F_2Be:FCl:$NHCH_2$	3.2	–0.5	–35.8		
F_2Be:FCl:NCH	2.0	–0.5	–9.9	–0.3	–8.8
F_2BeF^-	4.5	–0.3	–57.3	0.0	–53.1
Cl_2Be:FCl	1.2	–0.5	23.3	–0.2	23.9
Cl_2Be:FCl:NH_3	4.5	–0.4	–30.6		
Cl_2Be:FCl:$NHCH_2$			–36.4		
Cl_2Be:FCl:NCH	3.9	–0.5	–23.8		
Cl_2BeF^-	6.4	–0.3	–55.6	0.0	–49.5

Moiety	PSO	DSO	FC	SD	^1J(F-Cl)
F-Cl	642.0	0.1	–99.4	255.3	798.0
H_2Be:FCl	626.6	0.1	–94.4	252.0	784.4
HFBe:FCl (E)	632.4	0.1	–97.0	252.6	788.1
HFBe:FCl (Z)	629.6	0.1	–96.3	252.4	785.8
F_2Be:FCl	627.1	0.2	–101.5	251.0	776.8
Cl_2Be:FCl	615.5	0.2	–96.5	248.7	767.9
H_2Be:FCl:NH_3	199.7	0.1	294.2	68.7	562.8
HFBe:FCl:NH_3 (E)	192.3	0.1	293.9	63.8	550.2
HFBe:FCl:NH_3 (Z)	188.4	0.1	299.3	62.7	550.5
F_2Be:FCl:NH_3	172.3	0.2	322.7	54.7	549.8
Cl_2Be:FCl:NH_3	115.7	0.2	326.2		
H_2Be:FCl:$NHCH_2$	122.7	0.1	336.8	37.8	497.4
HFBe:FCl:$NHCH_2$ E	116.1	0.1	330.3	34.2	480.7
HFBe:FCl:$NHCH_2$ Z	111.2	0.1	329.2	32.6	473.1
F_2Be:FCl:$NHCH_2$	100.1	0.2	338.2		
Cl_2Be:FCl:$NHCH_2$			300.7		
H_2Be:FCl:NCH	432.3	0.1	54.3	175.7	662.5
HFBe:FCl:NCH (E)	431.7	0.2	49.3	173.3	654.5
HFBe:FCl:NCH (Z)	418.9	0.2	71.3	169.1	659.5
F_2Be:FCl:NCH	365.8	0.2	134.5	144.4	644.8
Cl_2Be:FCl:NCH	129.2	0.2	380.0		
FCl:NH_3	467.4	0.1	36.9	189.2	693.6
FCl:$NHCH_2$	440.7	0.1	60.0	178.8	679.6
FCl:NCH	578.6	0.1	–57.5	231.7	753.0

Moiety	PSO	DSO	FC	SD	^{1X}J(Cl-N)
FCl:NH3	–2.4	0.0	–48.2	–0.6	–51.1
H_2Be:FCl:NH_3	–5.9	0.0	–17.3	–2.7	–25.9
HFBe:FCl:NH_3 E	–6.0	0.0	–16.1	–2.8	–24.9
HFBe:FCl:NH_3 Z	–6.1	0.0	–14.7	–2.9	–23.7
F_2Be:FCl:NH_3	–6.3	0.0	–10.5	–3.0	–19.9
Cl_2Be:FCl:NH_3	–6.9	0.0	1.4		
H_3N-Cl^+	–8.8	0.0	21.7	–4.4	8.5
FCl:$NHCH_2$	–1.3	0.0	–54	–0.1	–55.4
H_2Be:FCl:$NHCH_2$	–1.7	0.0	6.5	–1.1	3.7
HFBe:FCl:$NHCH_2$ E	–1.7	0.0	7.8	–1.2	5.0
HFBe:FCl:$NHCH_2$ Z	–1.6	0.0	9.6	–1.1	6.8
F_2Be:FCl:$NHCH_2$	–1.6	0.2	12.6		
Cl_2Be:FCl:$NHCH_2$			20.4		
H_2C=(H)N-Cl^+	–4.1	0.0	27.9	–2.2	21.6
FCl:NCH	–0.4	0.0	–32.3	0.1	–32.7
H_2Be:FCl:NCH	–0.9	0.0	–57.2	0.1	–58.0
HFBe:FCl:NCH E	–0.9	0.0	–58.3	0.1	–59.1
HFBe:FCl:NCH Z	–0.9	0.0	–57.9	0.1	–58.7
F_2Be:FCl:NCH	–0.9	0.0	–54.2	0.1	–54.9
Cl_2Be:FCl:NCH	0.7	0.0	18.0		
HCN–Cl^+	0	0.0	48.6	0.3	48.8