

Supplementary Materials

Interplay between Beryllium Bonds and Anion- π Interactions in $\text{BeR}_2\text{:C}_6\text{X}_6\text{:Y}^-$ Complexes ($\text{R} = \text{H}, \text{F}$ and Cl , $\text{X} = \text{H}$ and F , and $\text{Y} = \text{Cl}$ and Br)

Table S1. Molecular graphs, MP2 energy (Hartree), Number of Imaginary Frequencies (NIMAG) and Cartesian coordinates ($\text{\AA}$) of C_6H_6 , $\text{C}_6\text{H}_6\text{:X}^-$, $\text{BeR}_2\text{:C}_6\text{H}_6$ and $\text{BeR}_2\text{:C}_6\text{H}_6\text{:X}^-$ systems.

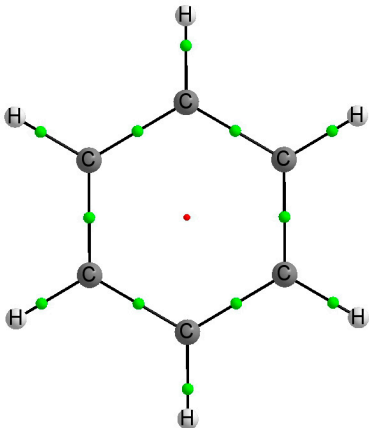
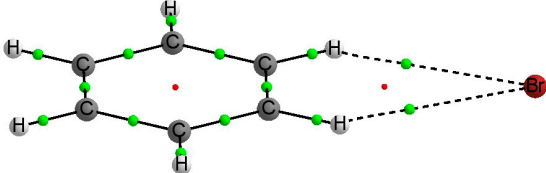
	C_6H_6 MP2 = -231.53535814 NIMAG = 0
	C, 0.0000000, 0.0000000, 1.4080620
	C, 1.2194175, 0.0000000, 0.7040310
	C, 1.2194175, 0.0000000, -0.7040310
	C, 0.0000000, 0.0000000, -1.4080620
	C, -1.2194175, 0.0000000, -0.7040310
	C, -1.2194175, 0.0000000, 0.7040310
	H, 0.0000000, 0.0000000, 2.5030653
	H, 2.1677182, 0.0000000, 1.2515327
	H, 2.1677182, 0.0000000, -1.2515327
	H, 0.0000000, 0.0000000, -2.5030653
	H, -2.1677182, 0.0000000, -1.2515327
	H, -2.1677182, 0.0000000, 1.2515327
	$\text{C}_6\text{H}_6\text{:Br}^-$ MP2 = -2804.15776381 NIMAG = 0
	C, -0.7043361781, 0., -2.5519491361
	C, -1.4057425715, 0., -1.3285831579
	C, -0.7045442698, 0., -0.1066306298
	C, 0.7045442698, 0., -0.1066306298
	C, 1.4057425715, 0., -1.3285831579
	C, 0.7043361781, 0., -2.5519491361
	H, -1.2524561776, 0., -3.5016246387
	H, -2.502071949, 0., -1.33007136
	H, -1.2144825587, 0., 0.863414021
	H, 1.2144825587, 0., 0.863414021
	H, 2.502071949, 0., -1.33007136
	H, 1.2524561776, 0., -3.5016246387
	Br, 0., 0., 3.4993293131

Table S1. *Cont.*

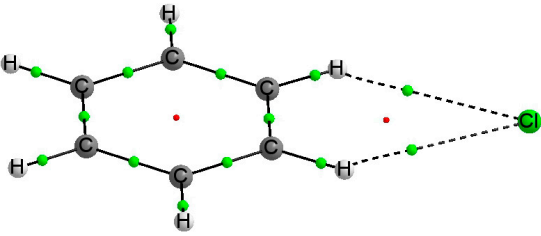
	C₆H₆:Cl⁻ MP2 = -691.27180164 NIMAG = 0 C, -0.7043236309, 0., -2.5396581427 C, -1.4058468748, 0., -1.3158622779 C, -0.7046877532, 0., -0.0939338865 C, 0.7046877532, 0., -0.0939338865 C, 1.4058468748, 0., -1.3158622779 C, 0.7043236309, 0., -2.5396581427 H, -1.2529266375, 0., -3.4892075267 H, -2.5023228441, 0., -1.3179720035 H, -1.2082109439, 0., 0.8798521549 H, 1.2082109439, 0., 0.8798521549 H, 2.5023228441, 0., -1.3179720035 H, 1.2529266375, 0., -3.4892075267 Cl, 0., 0., 3.3420028749
	C₆H₆:BeH₂ MP2 = -247.3635869 NIMAG = 0 C, 0.7521423406, -0.7647137121, 0.7015018414 C, 0.2112393693, 0.3212539413, 1.3998053119 C, -0.3261276451, 1.4046642969, 0.6987443107 C, -0.3261276451, 1.4046642969, -0.6987443107 C, 0.2112393693, 0.3212539413, -1.3998053119 C, 0.7521423406, -0.7647137121, -0.7015018414 H, 1.1882017202, -1.5996498902, 1.2420274688 H, 0.2115469181, 0.3218127011, 2.4858522813 H, -0.7494057432, 2.2448954459, 1.2412119946 H, -0.7494057432, 2.2448954459, -1.2412119946 H, 0.2115469181, 0.3218127011, -2.4858522813 H, 1.1882017202, -1.5996498902, -1.2420274688 Be, -1.4427582466, -2.2024622922, 0. H, -0.8148440282, -3.3852293633, 0. H, -2.3825565037, -1.2547419057, 0.

Table S1. *Cont.*

	Br⁻·C₆H₆·BeH₂ MP2 = -2819.99368763 NIMAG = 0 C, 0.6143364987, -1.1857977836, 0.7089752856 C, 0.3849145021, 0.019921447, 1.407666951 C, 0.1883244528, 1.2240942743, 0.7038536878 C, 0.1883244535, 1.224094274, -0.7038536885 C, 0.3849145036, 0.0199214463, -1.4076669509 C, 0.6143364995, -1.185797784, -0.7089752847 H, 0.8199460884, -2.1143749016, 1.2526227457 H, 0.380244482, 0.0171777073, 2.503221292 H, 0.0437223324, 2.1848099075, 1.211033786 H, 0.0437223337, 2.1848099069, -1.2110337873 H, 0.3802444846, 0.0171777062, -2.5032212919 H, 0.8199460897, -2.1143749021, -1.2526227442 Be, -1.4811721037, -1.80316123, -0.0000000005 H, -1.4112558474, -3.1719607293, -0.0000000001 H, -2.3018476673, -0.7236816858, -0.0000000012 Br, 0.2638909508, 4.7215260437, -0.0000000011
	Cl⁻·C₆H₆·BeH₂ MP2 = -707.10826090 NIMAG = 0 C, 0.611075753, -1.177151914, 0.7091039342 C, 0.3871789153, 0.0299684865, 1.4077934597 C, 0.1967698381, 1.2351691655, 0.7039847744 C, 0.1967698388, 1.2351691652, -0.7039847751 C, 0.3871789168, 0.0299684858, -1.4077934596 C, 0.6110757537, -1.1771519143, -0.7091039333 H, 0.8133964087, -2.1065595033, 1.2526929799 H, 0.3822096988, 0.0264932419, 2.5034490736 H, 0.0574851042, 2.2009483613, 1.2038946945 H, 0.0574851055, 2.2009483607, -1.2038946958 H, 0.3822097015, 0.0264932407, -2.5034490735 H, 0.8133964101, -2.1065595039, -1.2526929783 Be, -1.477440505, -1.7912996614, -0.0000000005 H, -1.4123400312, -3.1612012431, -0.0000000002 H, -2.3033351226, -0.7152816333, -0.0000000012 Cl, 0.2294762716, 4.5644305654, -0.0000000011

Table S1. *Cont.*

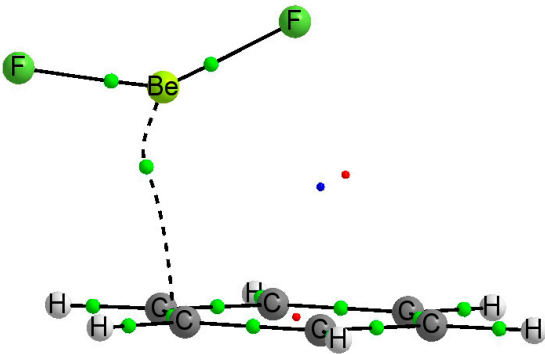
	C₆H₆:BeF₂ MP2 = −445.70937508 NIMAG = 0 C, 0.7166707495, −0.8217203662, 0.7093006754 C, 0.180940058, 0.2787240688, 1.4121529707 C, −0.3531693924, 1.369658695, 0.7038274062 C, −0.3531693924, 1.369658695, −0.7038274062 C, 0.180940058, 0.2787240688, −1.4121529707 C, 0.7166707495, −0.8217203662, −0.7093006754 H, 1.1540876782, −1.6672051414, 1.249520047 H, 0.1782936139, 0.2773802013, 2.5064693049 H, −0.7788101668, 2.2174729056, 1.2492279378 H, −0.7788101668, 2.2174729056, −1.2492279378 H, 0.1782936139, 0.2773802013, −2.5064693049 H, 1.1540876782, −1.6672051414, −1.249520047 Be, −1.1978989165, −1.9328295552, 0. F, −0.7199160246, −3.2949810578, 0. F, −2.3456180756, −1.0664263966, 0.
	Br[−]:C₆H₆:BeF₂ MP2 = −3018.34274853 NIMAG = 0 C, 0.5720275988, −1.162078929, 0.7109089689 C, 0.3636301155, 0.0486685803, 1.4103150182 C, 0.1781976206, 1.2508489409, 0.7050238187 C, 0.1781976206, 1.2508489409, −0.7050238197 C, 0.3636301155, 0.0486685803, −1.4103150192 C, 0.5720275988, −1.162078929, −0.7109089699 H, 0.7763216428, −2.092889539, 1.2509281188 H, 0.3625823261, 0.0467591397, 2.5054716337 H, 0.0519084187, 2.2151592623, 1.2101792984 H, 0.0519084187, 2.2151592623, −1.2101792994 H, 0.3625823261, 0.0467591397, −2.5054716347 H, 0.7763216428, −2.092889539, −1.2509281198 Be, −1.401943658, −1.8451798009, −0.0000000005 F, −1.2696511506, −3.3006638613, −0.0000000005 F, −2.4595153618, −0.8624628068, −0.0000000005 Br, 0.4543667674, 4.709755265, −0.0000000005

Table S1. *Cont.*

	Cl⁻:C₆H₆:BeF₂ MP2 = -905.45747792 NIMAG = 0 C, 0.5679499686, -1.1541837563, 0.7110385747 C, 0.3678982464, 0.0582859559, 1.4104763758 C, 0.1919784646, 1.2619184797, 0.7051743095 C, 0.1919784646, 1.2619184797, -0.7051743103 C, 0.3678982464, 0.0582859559, -1.4104763766 C, 0.5679499686, -1.1541837563, -0.7110385755 H, 0.7662870326, -2.0864945364, 1.2508408353 H, 0.3663754206, 0.0555859852, 2.5057367792 H, 0.0738269764, 2.2316692997, 1.2028262937 H, 0.0738269764, 2.2316692997, -1.2028262945 H, 0.3663754206, 0.0555859852, -2.5057367799 H, 0.7662870326, -2.0864945364, -1.250840836 Be, -1.4023168135, -1.8330114879, 0. F, -1.2758842719, -3.2899089973, -0.0000000004 F, -2.4636976162, -0.8536239067, -0.0000000004 Cl, 0.4058585485, 4.5573652369, -0.0000000004
	C₆H₆:BeCl₂ MP2 = -1165.69066708 NIMAG = 0 C, 0.7027531187, -0.8014838975, 0.7105341951 C, 0.1915448151, 0.3114543473, 1.4129667548 C, -0.3178392441, 1.4133996568, 0.7042289051 C, -0.3178392441, 1.4133996568, -0.7042289051 C, 0.1915448151, 0.3114543473, -1.4129667548 C, 0.7027531187, -0.8014838975, -0.7105341951 H, 1.142132852, -1.6453679079, 1.2519003756 H, 0.1888127275, 0.3099040859, 2.50732886 H, -0.7258920843, 2.2701193857, 1.2492078725 H, -0.7258920843, 2.2701193857, -1.2492078725 H, 0.1888127275, 0.3099040859, -2.50732886 H, 1.142132852, -1.6453679079, -1.2519003756 Be, -1.141695336, -1.9669981768, 0. Cl, -0.5641482233, -3.7464465493, 0. Cl, -2.7245887659, -0.9882229095, 0.

Table S1. *Cont.*

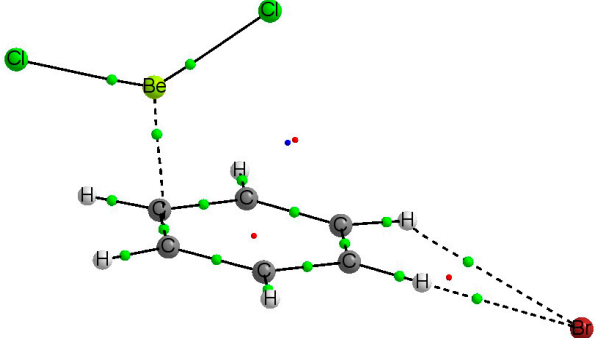
	Br⁻·C₆H₆·BeCl₂ MP2 = -3738.32736513 NIMAG = 0 C, 0.2462707594, -2.4668938711, 0.7125263697 C, 0.2503060592, -1.2372008349, 1.4109852598 C, 0.2802691664, -0.021318536, 0.7051763991 C, 0.2802691664, -0.021318536, -0.7051763991 C, 0.2503060592, -1.2372008349, -1.4109852598 C, 0.2462707594, -2.4668938711, -0.7125263697 H, 0.3094095061, -3.4170219407, 1.253826336 H, 0.2458804725, -1.239293931, 2.5060985854 H, 0.3277443299, 0.9507571156, 1.2092772003 H, 0.3277443299, 0.9507571156, -1.2092772003 H, 0.2458804725, -1.239293931, -2.5060985854 H, 0.3094095061, -3.4170219407, -1.253826336 Be, -1.7663301992, -2.8127362721, 0. Cl, -2.0227005771, -4.6993106303, 0. Cl, -2.9758611022, -1.3825599629, 0. Br, 1.2581352555, 3.2726088799, 0.
	Cl⁻·C₆H₆·BeCl₂ MP2 = -1625.44225034 NIMAG = 0 C, 0.5153501772, -1.6793031196, 0.7126802469 C, 0.509107463, -0.4493149224, 1.4111056511 C, 0.5298596868, 0.7668739951, 0.7053200961 C, 0.5298596868, 0.7668739951, -0.7053200961 C, 0.509107463, -0.4493149224, -1.4111056511 C, 0.5153501772, -1.6793031196, -0.7126802469 H, 0.5872571489, -2.6289614866, 1.2538370174 H, 0.504256828, -0.4521486724, 2.5063142824 H, 0.5715441462, 1.7436364666, 1.2018844631 H, 0.5715441462, 1.7436364666, -1.2018844631 H, 0.504256828, -0.4521486724, -2.5063142824 H, 0.5872571489, -2.6289614866, -1.2538370174 Be, -1.4876935801, -2.0484364068, 0. Cl, -1.7256923505, -3.939047462, 0. Cl, -2.7198318552, -0.6369351834, 0. Cl, 1.354993898, 3.9314305306, 0.

Table S2. Molecular graphs, MP2 energy (Hartree), Number of Imaginary Frequencies (NIMAG) and Cartesian coordinates (Å) of C_6F_6 , $C_6F_6: X^-$, $BeR_2:C_6F_6$ and $BeR_2:C_6F_6:X^-$ systems.

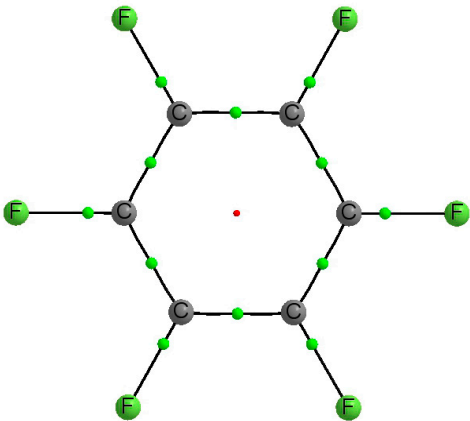
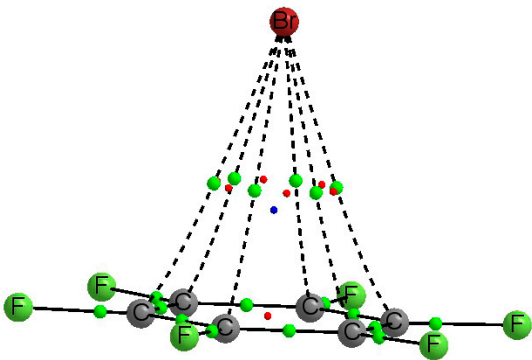
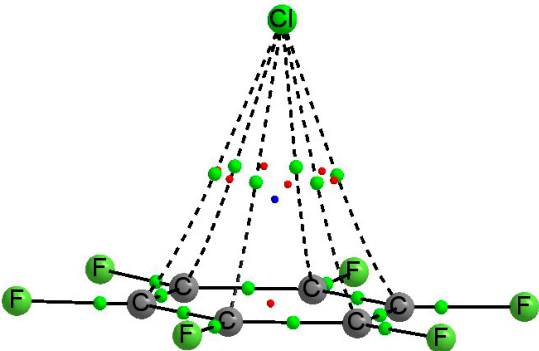
	C_6F_6 MP2 = -825.83972849 NIMAG = 0 C, 0.911266765, -0.759597649, 0.7005947318 C, 0.264231777, 0.2670822926, 1.4009370781 C, -0.3829084153, 1.2937445447, 0.7006019122 C, -0.382908446, 1.2937445939, -0.7006018115 C, 0.2642317155, 0.267082391, -1.4009370779 C, 0.9112667343, -0.7595975998, -0.7005948322 F, 1.5328927352, -1.7454932278, 1.3737129125 F, 0.2648272056, 0.2674178633, 2.7471162288 F, -1.0035359371, 2.2802746733, 1.3739028022 F, -1.0035359974, 2.2802747698, -1.3739026049 F, 0.2648270851, 0.2674180564, -2.7471162286 F, 1.5328926749, -1.7454931313, -1.3737131095
	$C_6F_6:Br^-$ MP2 = -3398.47408565 NIMAG = 0 C, 1.3969839, 0.0000000, 0.0000000 C, 0.6984919, -1.2098235, 0.0000000 C, -0.6984919, -1.2098235, 0.0000000 C, -1.3969839, 0.0000000, 0.0000000 C, -0.6984919, 1.2098235, 0.0000000 C, 0.6984919, 1.2098235, 0.0000000 F, 2.7485503, 0.0000000, -0.0202356 F, 1.3742752, -2.3803144, -0.0202356 F, -1.3742752, -2.3803144, -0.0202356 F, -2.7485503, 0.0000000, -0.0202356 F, -1.3742752, 2.3803144, -0.0202356 F, 1.3742752, 2.3803144, -0.0202356 Br, 0.0000000, 0.0000000, -3.2133507
	$C_6F_6:Cl^-$ MP2 = -1285.58803712 NIMAG = 0 C, 1.3966363, 0.0000000, 0.0000000 C, 0.6983182, -1.2095225, 0.0000000 C, -0.6983182, -1.2095225, 0.0000000 C, -1.3966363, 0.0000000, 0.0000000 C, -0.6983182, 1.2095225, 0.0000000 C, 0.6983182, 1.2095225, 0.0000000 F, 2.7489492, 0.0000000, -0.0197052 F, 1.3744746, -2.3806599, -0.0197052 F, -1.3744746, -2.3806599, -0.0197052 F, -2.7489492, 0.0000000, -0.0197052 F, -1.3744746, 2.3806599, -0.0197052 F, 1.3744746, 2.3806599, -0.0197052 Cl, 0.0000000, 0.0000000, -3.0639319

Table S2. *Cont.*

	Br⁻:C₆F₆:BeH₂ MP2 = -3414.30430516 NIMAG = 0 C, 0.1325222684, -1.1116544707, 0.702815867 C, 0.0764975044, 0.1043032811, 1.3980356454 C, 0.0392036586, 1.3131876001, 0.6976905227 C, 0.0392036586, 1.3131876001, -0.6976905227 C, 0.0764975044, 0.1043032811, -1.3980356454 C, 0.1325222684, -1.1116544707, -0.702815867 F, 0.2786965048, -2.2633028905, 1.376666024 F, 0.1041717192, 0.1068397837, 2.7445041517 F, -0.0087059004, 2.4797332342, 1.372548301 F, -0.0087059004, 2.4797332342, -1.372548301 F, 0.1041717192, 0.1068397837, -2.7445041517 F, 0.2786965048, -2.2633028905, -1.376666024 Be, -2.2805353226, -1.0724085638, 0. H, -2.4485183431, -2.4139684674, 0. H, -2.676776158, 0.2200059575, 0. Br, 3.2277988126, -0.283545328, 0.
	Cl⁻:C₆F₆:BeH₂ MP2 = -1301.41866829 NIMAG = 0 C, 0.1445888962, -1.1051154971, 0.7027465033 C, 0.0824670651, 0.110441153, 1.3977432539 C, 0.0421894986, 1.3190078102, 0.6976179087 C, 0.0421894986, 1.3190078102, -0.6976179087 C, 0.0824670651, 0.110441153, -1.3977432539 C, 0.1445888962, -1.1051154971, -0.7027465033 F, 0.298036247, -2.2553943846, 1.3765973198 F, 0.1101595374, 0.1132640697, 2.7447505612 F, -0.0126336511, 2.4861760477, 1.3726962865 F, -0.0126336511, 2.4861760477, -1.3726962865 F, 0.1101595374, 0.1132640697, -2.7447505612 F, 0.298036247, -2.2553943846, -1.3765973198 Be, -2.251188797, -1.0764293964, 0. H, -2.4264909177, -2.4180009492, 0. H, -2.6640428726, 0.2117468799, 0. Cl, 3.0788479152, -0.3457782566, 0.

Table S2. *Cont.*

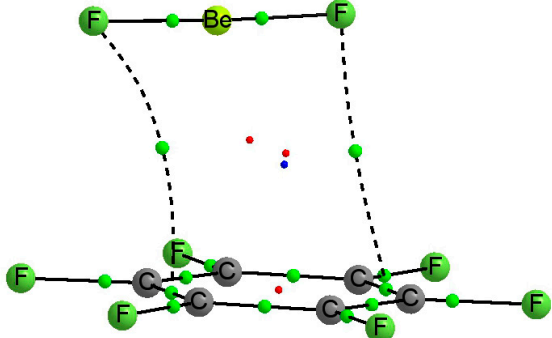
	C₆F₆:BeF₂ MP2 = −1040.00401005 NIMAG = 0 C, 0.8413256116, −0.9062017651, 0.6023779626 C, 0.4637216482, 0.2178852601, 1.3546486432 C, 0.1419319966, 1.4204558315, 0.7094893294 C, 0.1909799019, 1.5022060413, −0.687686493 C, 0.5646390283, 0.3825414195, −1.441299043 C, 0.8869090959, −0.8212163145, −0.7986087982 F, 1.194536075, −2.0429626217, 1.2203422276 F, 0.4253419748, 0.1437383079, 2.6978675515 F, −0.2324316835, 2.4894664003, 1.4334722934 F, −0.1434566924, 2.6464290677, −1.3055768469 F, 0.5962837279, 0.4545533931, −2.7832611239 F, 1.2550205345, −1.8935514038, −1.5237543341 Be, −2.0853864971, −1.2210304403, 0.1788243737 F, −1.780716965, −2.4426873601, 0.8292303594 F, −2.4444037567, −0.012161816, −0.4760661018
	Br[−]:C₆F₆:BeF₂ MP2 = −3612.65022072 NIMAG = 0 C, 0.1175083571, −1.1030326408, 0.704912836 C, 0.0816924121, 0.1152730641, 1.4006026026 C, 0.0399785231, 1.3210574958, 0.6985665022 C, 0.0399785231, 1.3210574958, −0.6985665022 C, 0.0816924121, 0.1152730641, −1.4006026026 C, 0.1175083571, −1.1030326408, −0.704912836 F, 0.2712721807, −2.2535587444, 1.3739535881 F, 0.1090021549, 0.1168356143, 2.7451182064 F, −0.0154584213, 2.4871618492, 1.3692553835 F, −0.0154584213, 2.4871618492, −1.3692553835 F, 0.1090021549, 0.1168356143, −2.7451182064 F, 0.2712721807, −2.2535587444, −1.3739535881 Be, −2.1518988504, −1.0683494636, 0. F, −2.4339913316, −2.4787349453, 0. F, −2.7407676204, 0.2480277751, 0. Br, 3.1854078613, −0.3601199714, 0.

Table S2. *Cont.*

	Cl⁻:C₆F₆:BeF₂ MP2 = -1499.76478931 NIMAG = 0 C, 0.1304599769, -1.0981975014, 0.7048033292 C, 0.088693543, 0.1197124033, 1.4003316349 C, 0.0448868971, 1.3251720136, 0.698525503 C, 0.0448868971, 1.3251720136, -0.698525503 C, 0.088693543, 0.1197124033, -1.4003316349 C, 0.1304599769, -1.0981975014, -0.7048033292 F, 0.2896186333, -2.2476259334, 1.3739267917 F, 0.1158482911, 0.1215292413, 2.7454292226 F, -0.0169578944, 2.4918652088, 1.3694522828 F, -0.0169578944, 2.4918652088, -1.3694522828 F, 0.1158482911, 0.1215292413, -2.7454292226 F, 0.2896186333, -2.2476259334, -1.3739267917 Be, -2.1304688645, -1.0703623802, 0. F, -2.4144496363, -2.4813708572, 0. F, -2.7330534999, 0.24080587, 0. Cl, 3.0396136126, -0.405686823, 0.
	C₆F₆:BeCl₂ MP2 = -1759.98660426 NIMAG = 0 C, 0.9645201323, -0.7349155382, 0.7019134407 C, 0.3123253396, 0.2908251057, 1.4010614028 C, -0.3357499052, 1.3163936209, 0.7001087293 C, -0.3357499052, 1.3163936209, -0.7001087296 C, 0.3123253396, 0.2908251057, -1.401061403 C, 0.9645201323, -0.7349155382, -0.7019134409 F, 1.6092532906, -1.703857947, 1.3740803599 F, 0.3023081338, 0.2847141677, 2.746919026 F, -0.9823339387, 2.284490655, 1.372184801 F, -0.9823339387, 2.284490655, -1.3721848012 F, 0.3023081338, 0.2847141677, -2.7469190263 F, 1.6092532906, -1.703857947, -1.3740803602 Be, -1.9228060303, -2.1447975785, 0. Cl, -0.8844943869, -3.6335273126, 0. Cl, -3.000334999, -0.6795467166, 0.

Table S2. *Cont.*

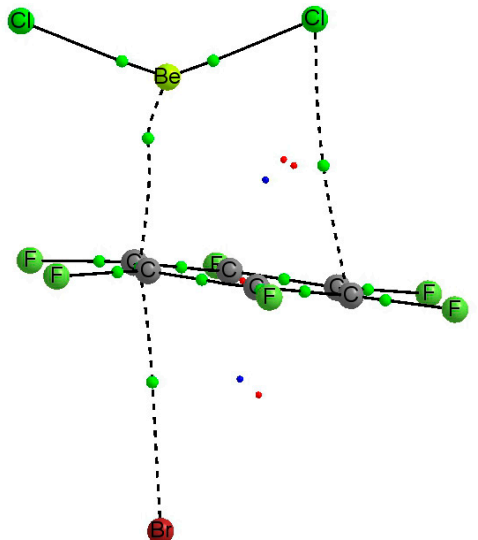
	Br⁻:C₆F₆:BeCl₂ MP2 = -4332.6331655 NIMAG = 0 C, 0.1283133987, -1.0853669684, 0.7064373673 C, 0.1052101693, 0.1350343736, 1.4014736923 C, 0.082866932, 1.3405356251, 0.698911173 C, 0.082866932, 1.3405356251, -0.698911173 C, 0.1052101693, 0.1350343736, -1.4014736923 C, 0.1283133987, -1.0853669684, -0.7064373673 F, 0.3094124745, -2.2299383801, 1.3752078145 F, 0.1310269603, 0.1364877611, 2.7442515454 F, 0.0379973611, 2.5065099727, 1.3676376433 F, 0.0379973611, 2.5065099727, -1.3676376433 F, 0.1310269603, 0.1364877611, -2.7442515454 F, 0.3094124745, -2.2299383801, -1.3752078145 Be, -2.1244769969, -1.1047308233, 0. Cl, -2.5334123442, -2.9202010207, 0. Cl, -3.0423786912, 0.5236600905, 0. Br, 3.1773539172, -0.3969563438, 0.
	Cl⁻:C₆F₆:BeCl₂ MP2 = -2219.7479135 NIMAG = 0 C, 0.1420374244, -1.0806260026, 0.706333468 C, 0.1118848184, 0.13947003, 1.4011786125 C, 0.0877376737, 1.3447296534, 0.6989006523 C, 0.0877376737, 1.3447296534, -0.6989006523 C, 0.1118848184, 0.13947003, -1.4011786125 C, 0.1420374244, -1.0806260026, -0.706333468 F, 0.3284751274, -2.2238569548, 1.3750119752 F, 0.1367960727, 0.141077959, 2.7445470619 F, 0.0359995096, 2.5112623732, 1.3678500823 F, 0.0359995096, 2.5112623732, -1.3678500823 F, 0.1367960727, 0.141077959, -2.7445470619 F, 0.3284751274, -2.2238569548, -1.3750119752 Be, -2.1003024349, -1.1050845722, 0. Cl, -2.5142391854, -2.9213393894, 0. Cl, -3.0348529958, 0.515860785, 0. Cl, 3.0302738505, -0.4452542688, 0.

Table S3. HOMA aromaticity index.

System	Homa Index	System	HOMA index
C_6H_6	1.00	C_6F_6	0.99
$BeH_2:C_6H_6$	1.00	$BeF_2:C_6F_6$	0.99
$BeF_2:C_6H_6$	0.99	$BeF_2:C_6F_6$	0.99
$BeCl_2:C_6H_6$	0.99	$BeCl_2:C_6F_6$	0.99
$C_6H_6:Br^-$	1.00	$C_6F_6:Br^-$	0.97
$C_6H_6:Cl^-$	1.00	$C_6F_6:Cl^-$	0.97
$BeH_2:C_6H_6:Br^-$	0.99	$BeH_2:C_6F_6:Br^-$	0.98
$BeH_2:C_6H_6:Cl^-$	0.99	$BeH_2:C_6F_6:Cl^-$	0.98
$BeF_2:C_6H_6:Br^-$	0.99	$BeF_2:C_6F_6:Br^-$	0.98
$BeF_2:C_6H_6:Cl^-$	0.99	$BeF_2:C_6F_6:Cl^-$	0.98
$BeCl_2:C_6H_6:Br^-$	0.98	$BeCl_2:C_6F_6:Br^-$	0.98
$BeCl_2:C_6H_6:Cl^-$	0.98	$BeCl_2:C_6F_6:Cl^-$	0.98