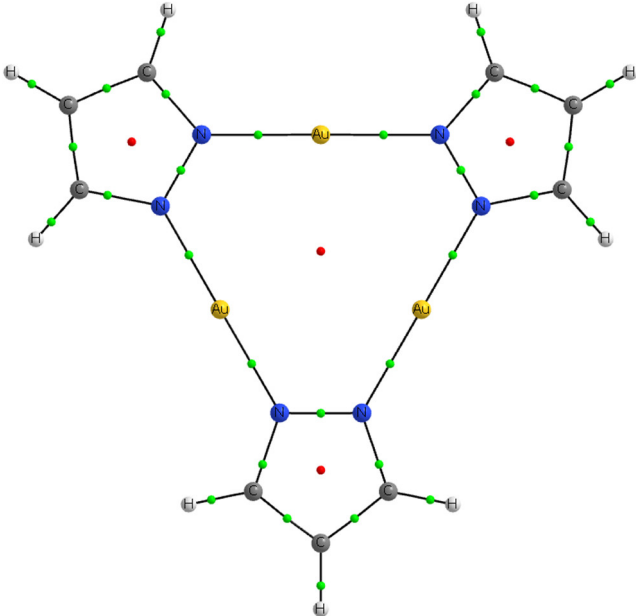


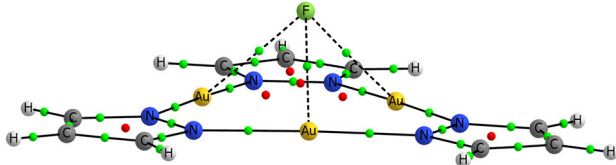
A Computational Study of the Interaction of Trinuclear Regium Complexes of Pyrazolate with Anions

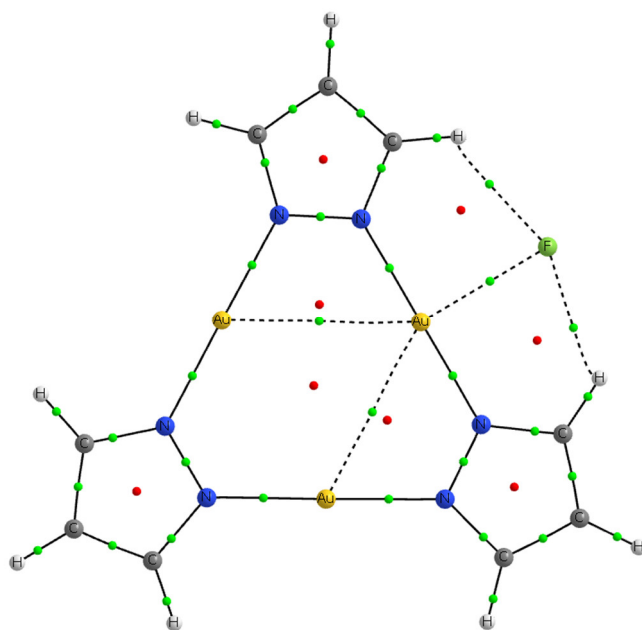
Ibon Alkorta, José Elguero, Cristina Trujillo and Goar Sánchez-Sanz

Pg. S2-19	Table S1. Molecular graph, electronic energy and geometry of the $(\text{Pz-Au})_3\text{:X}^{-\text{n}}$ complexes
Pg. S20-43	Table S2. Molecular graph, electronic energy and geometry of the $(\text{Pz-Ag})_3\text{:X}^{-\text{n}}$ complexes
Pg. S44-65	Table S3. Molecular graph, electronic energy and geometry of the $(\text{Pz-Cu})_3\text{:X}^{-\text{n}}$ complexes
Pg. S66-67	Table S4. Electron density properties at the intermolecular BCPs in the 1:1 complexes.
Pg. S68	Table S5. Barriers (kJ mol^{-1}) and interhalogen distance (\AA) in the maximum of the dissociation curve (Fig. S1) of the 1:2 apical complexes.
Pg. S69	Table S6. Interatomic distances (\AA) of the anions in the 1:2 complexes.
Pg. S70	Table S7. Anion-Anion repulsion corrected binding energies (kJ mol^{-1}) in the 1:2 complexes.
Pg. S71-72	Table S8. Electron density properties at the intermolecular BCPs in the 1:2 complexes.
Pg. S73	Table S9. Interatomic distances (\AA) of the anions in the 1:3 complexes.
Pg. S74	Table S10. Anion-Anion repulsion corrected binding energies (kJ/mol) in the 1:3 complexes.
Pg. S75	Table S11. Electron density properties at the intermolecular BCPs in the 1:3 complexes.
Pg. S76	Table S12. Anion-Metal distances in the CSD search.
Pg. S77.	Figure S1. Energy profiles (kJ mol^{-1}) as a function of the X-X distance (\AA) in the 1:2 apical complexes. Only one of the X anions in move further away from the $(\text{Pz-M})_3$ system.
Pg. S78-79	Figure S2. Electron density at the BCP (au) vs. the interatomic distance (\AA).

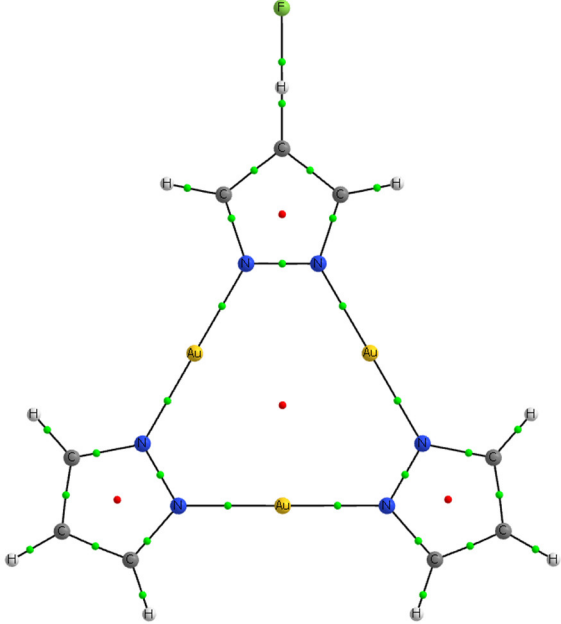
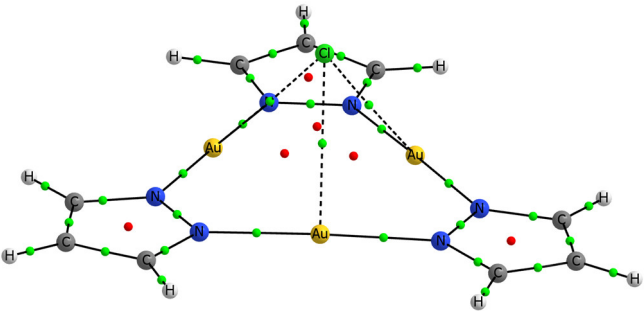
Table S1. Molecular graph, electronic energy and geometry of the (Pz-Au)₃:X⁻_n complexes.

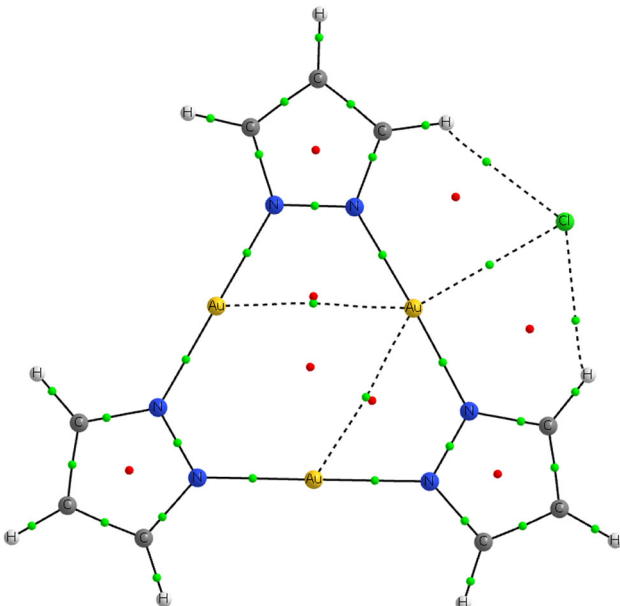
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	H,15,r2011,9,a20115,4,180.,0
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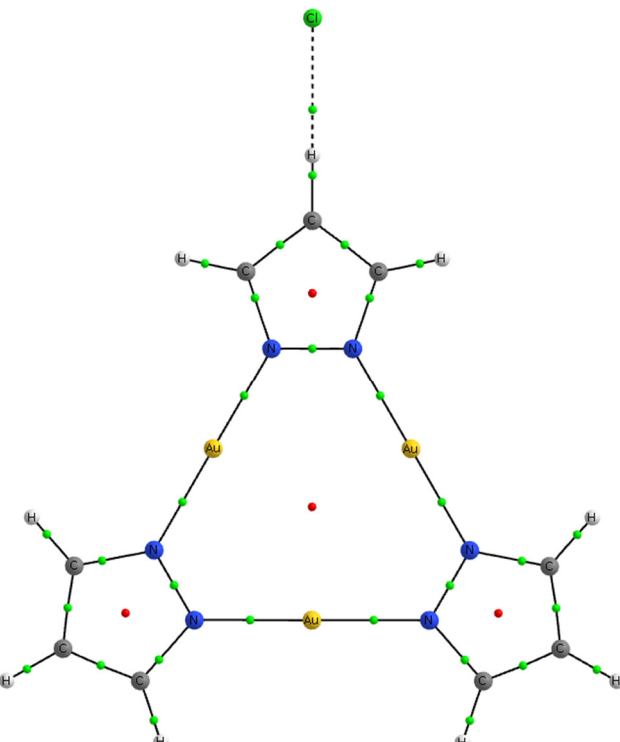
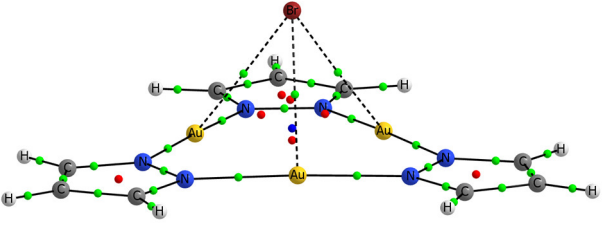
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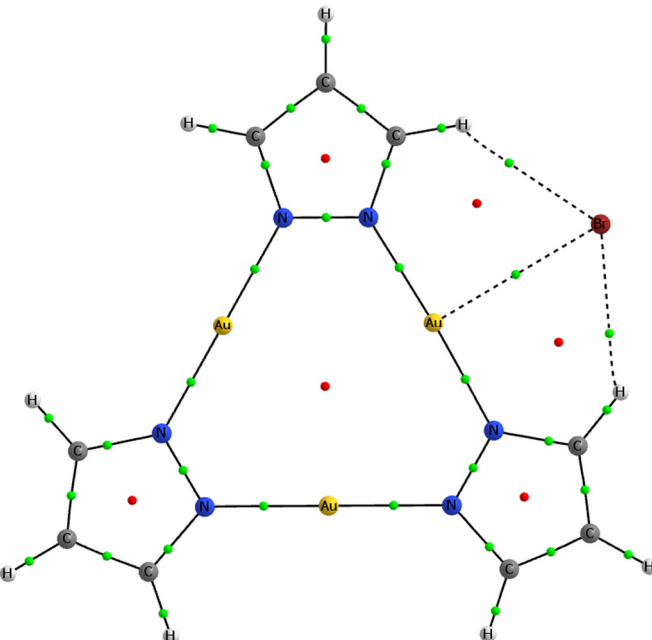


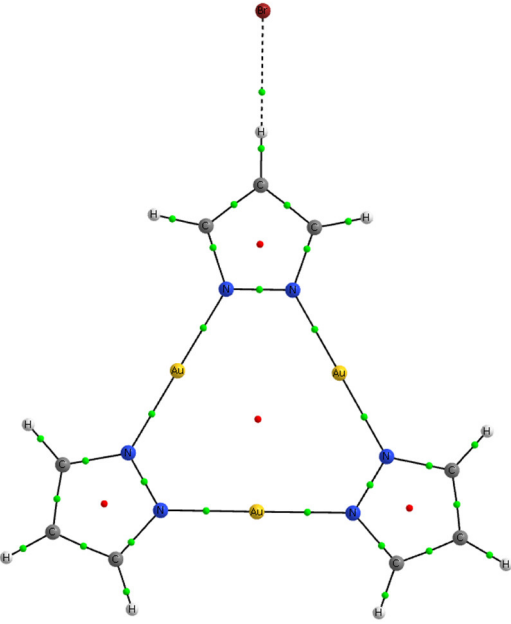
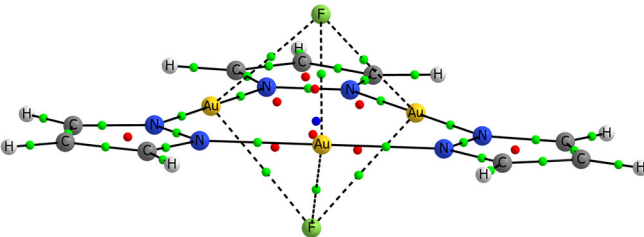
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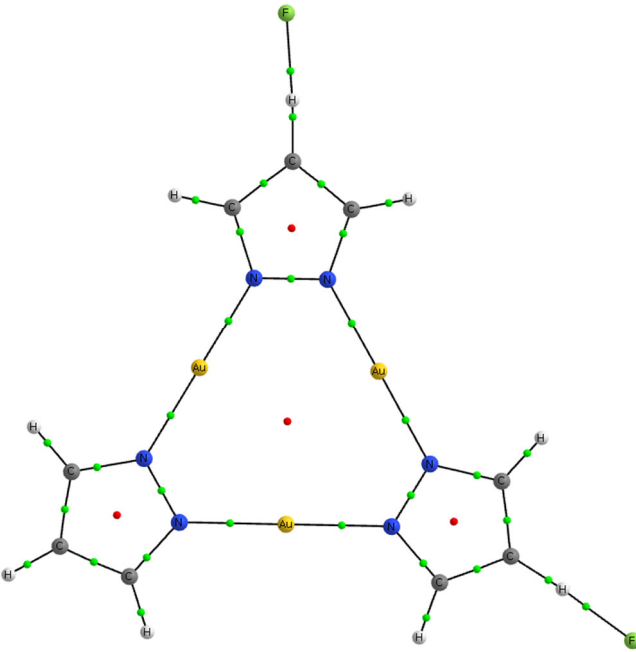
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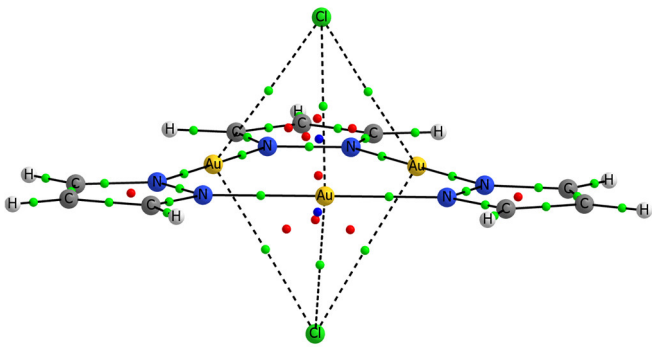
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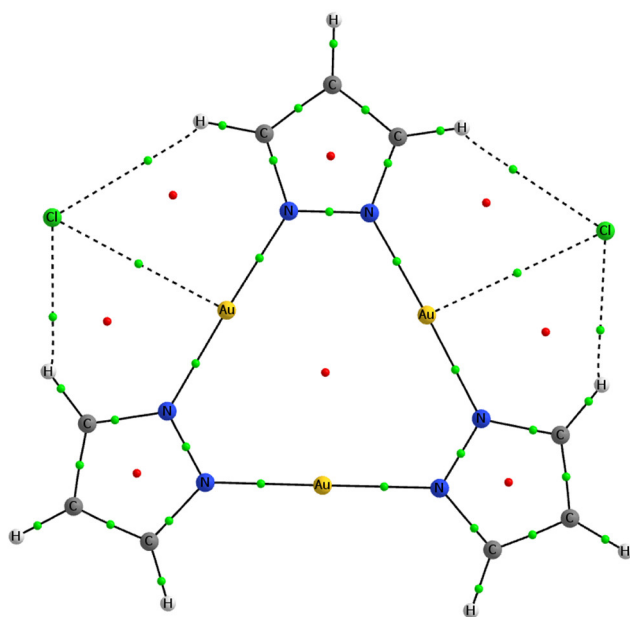
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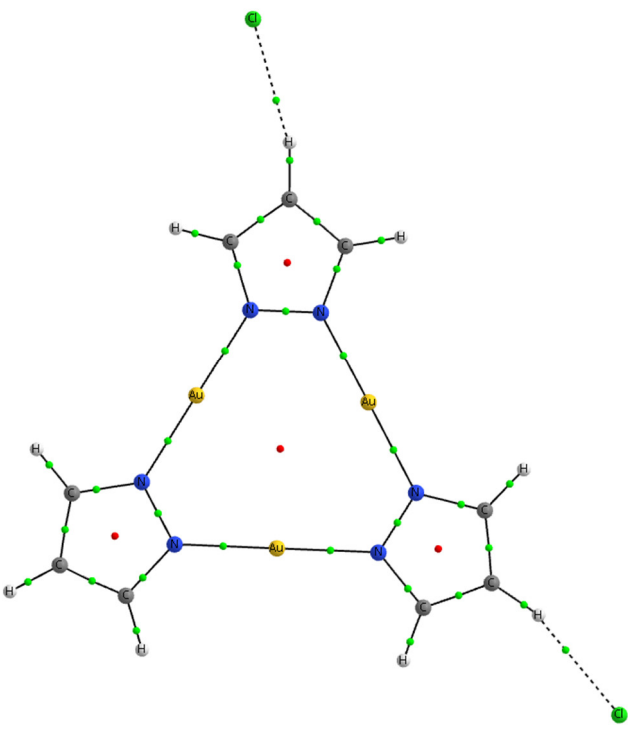
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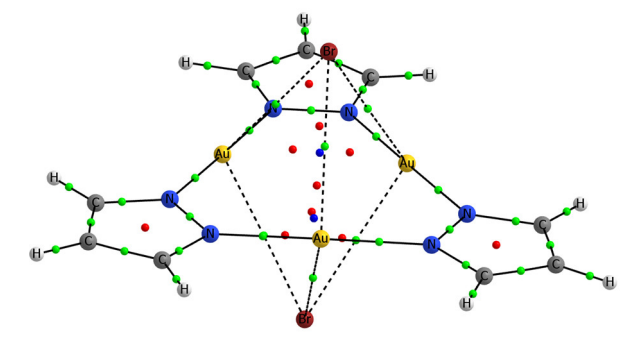
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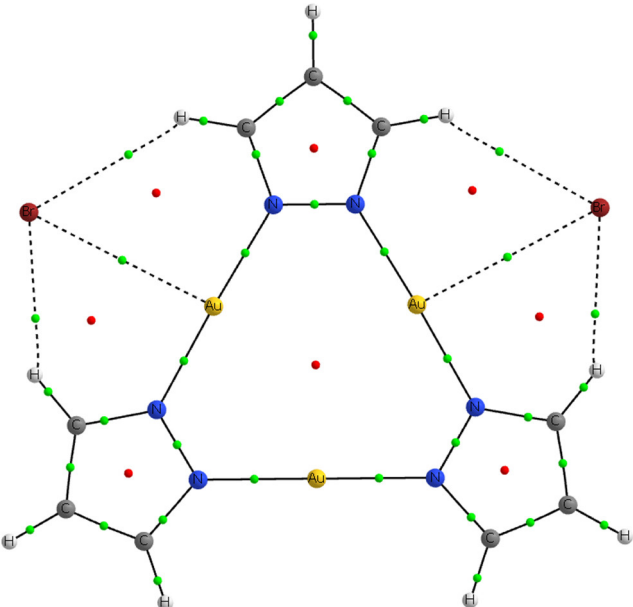
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	C,-2.8824058055,-0.0000449124,-2.9511863222
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	C,-4.1856420839,-0.0002920691,-2.4165735405
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	H,-2.1833185108,-0.0000770926,4.1781300793
	H,4.7100585622,-0.0000800736,-0.1982735793
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	H,5.1296989183,-0.0006137176,-2.9616430653
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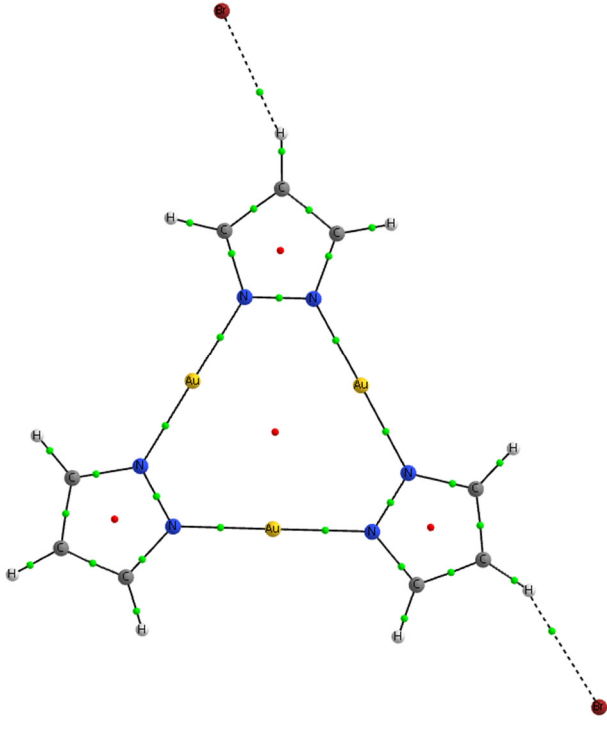


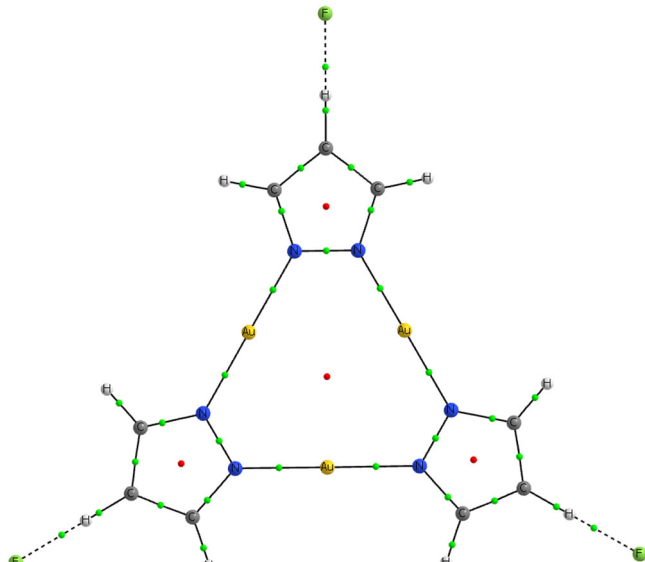
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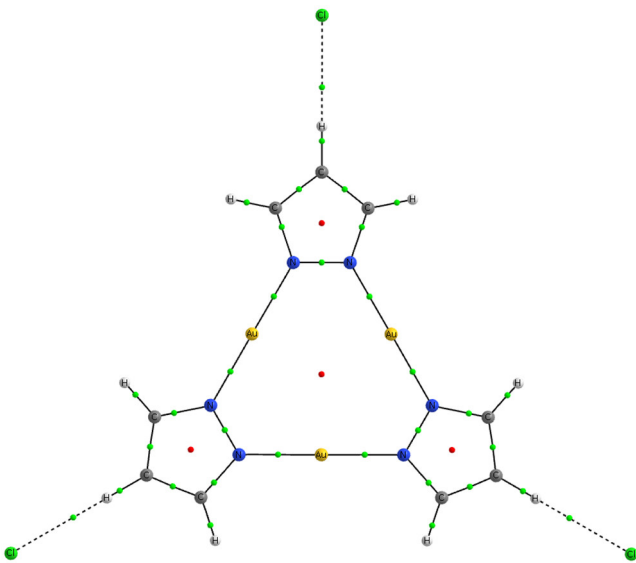
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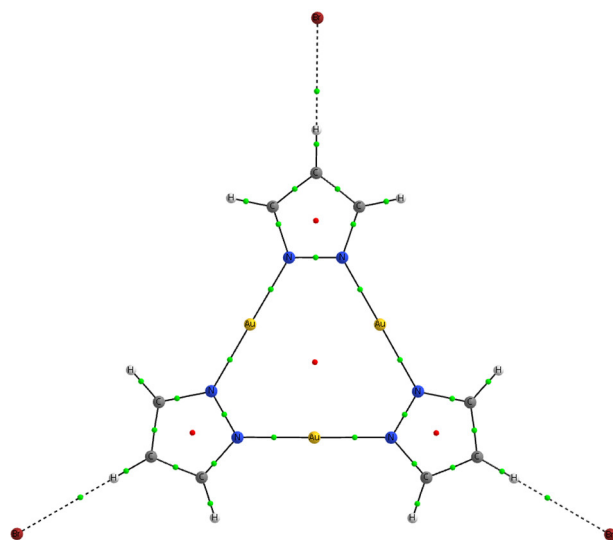
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	<p> Au,1.6909096052,0.,0.9775995718 Au,-0.0011712613,0.,-1.9531704595 Au,-1.6658560965,0.,0.9617824657 Br,4.6071927542,0.,2.8308873143 Br,-0.1480239522,0.,-5.4053896224 </p>
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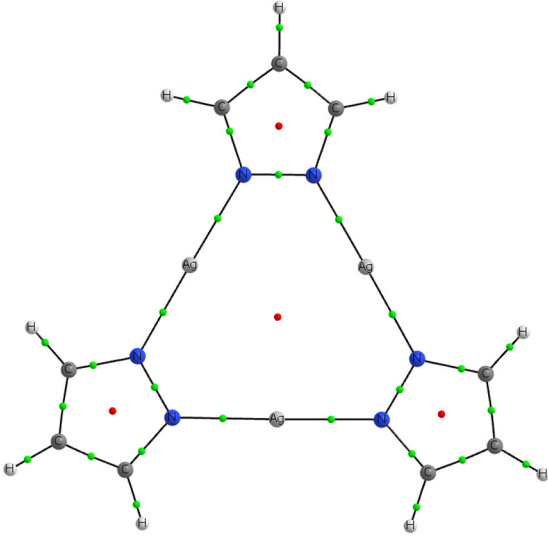
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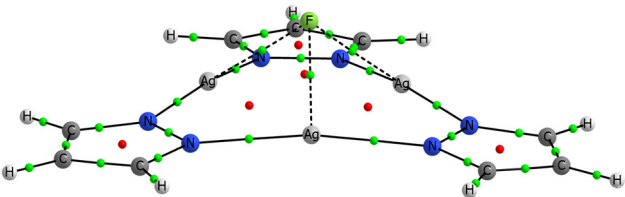
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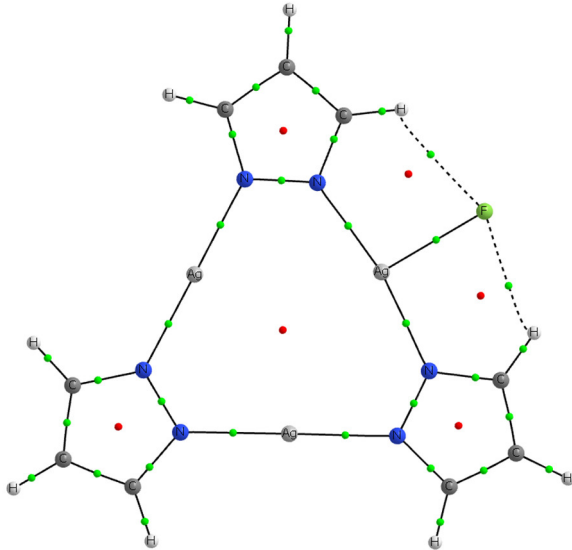


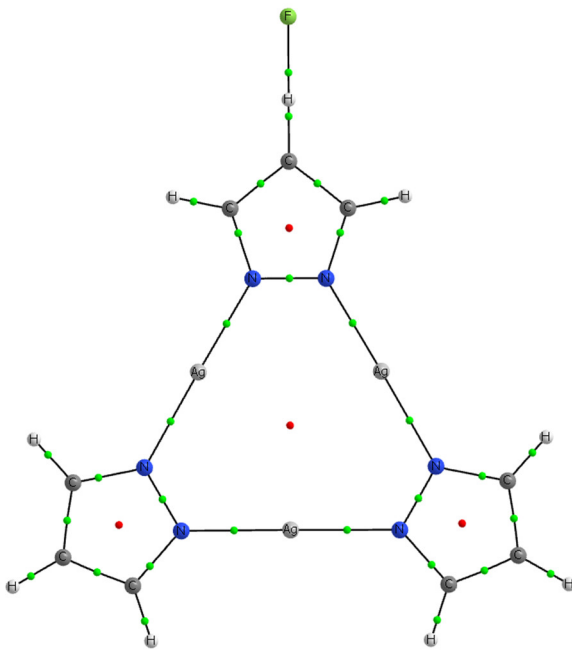
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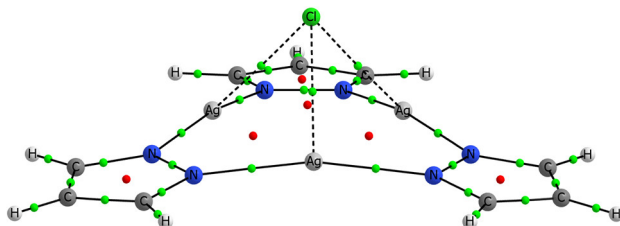
Table S2. Molecular graph, electronic energy and geometry of the (Pz-Ag)₃:X⁻ⁿ complexes.

	MP2= -1114.42179833 NIMAG= 0
	X
	X,1,r21
	X,1,r21,2,120.
	X,1,r21,2,120.,3,180.,0
	N,2,r52,1,90.,3,0.,0
	N,2,r52,1,90.,4,0.,0
	N,3,r52,1,90.,2,0.,0
	N,3,r52,1,90.,4,0.,0
	N,4,r52,1,90.,3,0.,0
	N,4,r52,1,90.,2,0.,0
	C,5,r115,2,a1152,1,180.,0
	C,6,r115,2,a1152,1,180.,0
	C,7,r115,3,a1152,1,180.,0
	C,8,r115,3,a1152,1,180.,0
	C,9,r115,4,a1152,1,180.,0
	C,10,r115,4,a1152,1,180.,0
	C,1,r171,3,120.,2,0.,0
	C,1,r171,4,120.,3,0.,0
	C,1,r171,2,120.,4,0.,0
	H,11,r2011,5,a20115,2,180.,0
	H,12,r2011,6,a20115,2,180.,0
	H,13,r2011,7,a20115,3,180.,0
	H,14,r2011,8,a20115,3,180.,0
	H,15,r2011,9,a20115,4,180.,0
	H,16,r2011,10,a20115,4,180.,0
	H,1,r261,3,120.,2,0.,0
	H,1,r261,4,120.,3,0.,0
	H,1,r261,2,120.,4,0.,0
	Ag,1,r291,3,60.,2,0.,0
	Ag,1,r291,4,60.,3,0.,0
	Ag,1,r291,2,60.,4,0.,0
	r21=2.7498381
	r52=0.68417589
	r115=1.36645246
	r171=4.90601527
	r2011=1.08948985
	r261=5.99465491
	r291=1.97902891
	a1152=108.26155634
	a20115=120.12601866

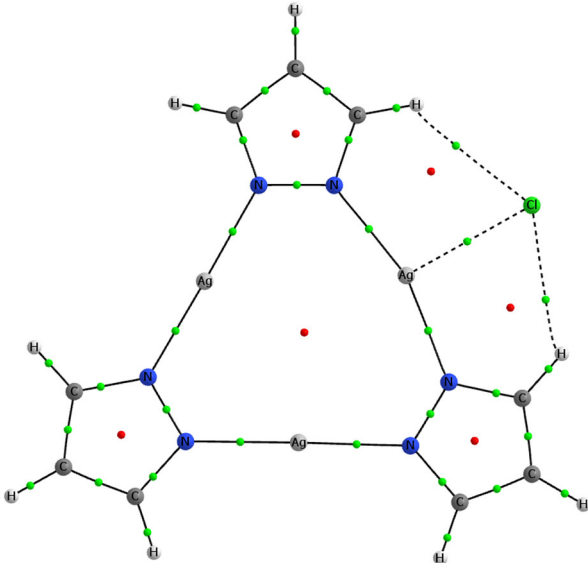
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	N,-
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	N,2.7707743953,-
	0.8092817168,0.0421704776
	N,2.0862473603,-
	1.994918628,0.0421709719
	N,-2.0862471865,-
	1.9949205114,0.0421687052
	N,-2.7707745391,-
	0.8092833154,0.0421703206
	C,1.1110672261,4.0981657838,0.137400929
	9
	C,-
	1.1110666698,4.0981647808,0.137418986
	C,4.1046491968,-
	1.0868701725,0.1374066072
	C,2.9935817886,-
	3.0112944084,0.1374181977
	C,-2.9935828094,-
	3.011295924,0.1374074125
	C,-4.1046495614,-
	1.086870289,0.1374051493
	C,0.0000001169,4.9617570267,0.197524789
	9
	C,4.2970081392,-
	2.4808783707,0.1975225257
	C,-4.2970086809,-
	2.4808786975,0.1975172272
	H,2.1784734139,4.3185487358,0.15616053
	31
	H,-
	2.1784728878,4.3185464551,0.156196709
	H,4.8292091753,-
	0.2726606238,0.156170899
	H,2.6507349467,-
	4.0458862111,0.1561942778
	H,-2.6507367519,-
	4.045888069,0.1561776038

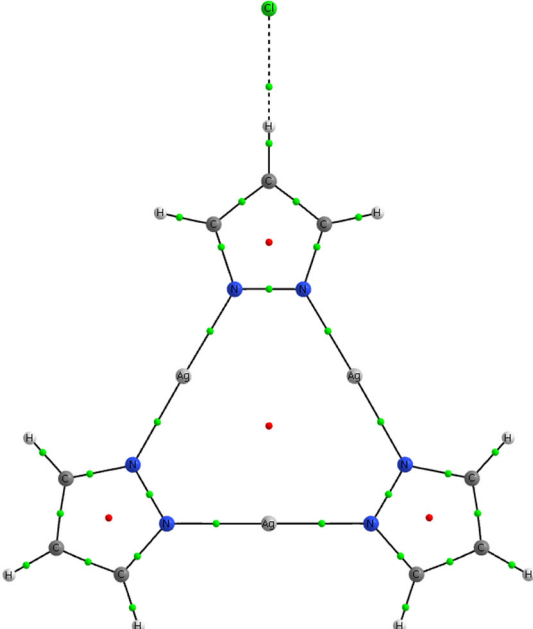
	H,-4.8292089073,- 0.2726601621,0.1561734535 H,-0.00000013,6.0491520773,0.2722216543 H,5.2387199518,- 3.0245760572,0.272217255 H,-5.2387207482,- 3.0245759886,0.2722112075 Ag,1.6702750741,0.9643341767,- 0.1147617396 Ag,0.0000003317,-1.928665709,- 0.1147559912 Ag,-1.6702723759,0.9643322821,- 0.1147530868 F,-0.0000017587,-0.000000671,- 1.5068433766
	MP2= -1214.14614086 NIMAG= 0 N,-0.6834987362,0.,-2.9761170683 N,0.6834987362,0.,-2.9761170683 N,-2.821161438,0.,0.5078527881 N,-2.0678216748,0.,1.6492588191 N,2.0678216748,0.,1.6492588191 N,2.821161438,0.,0.5078527881 C,-1.1115199447,0.,-4.2736926823 C,1.1115199447,0.,-4.2736926823 C,-4.1441178715,0.,0.8617716116 C,-2.9060491826,0.,2.7228451794 C,2.9060491826,0.,2.7228451794 C,4.1441178715,0.,0.8617716116 C,0.,0.,-5.135767117 C,-4.2407397777,0.,2.2665202801 C,4.2407397777,0.,2.2665202801 H,-2.178578322,0.,-4.4944663742 H,2.178578322,0.,-4.4944663742 H,-4.9188089716,0.,0.0942224103 H,-2.4553216712,0.,3.7178573913 H,2.4553216712,0.,3.7178573913 H,4.9188089716,0.,0.0942224103 H,0.,0.,-6.2249525323 H,-5.1509032781,0.,2.8659655643 H,5.1509032781,0.,2.8659655643 Ag,-1.7507342177,0.,-1.2233459218 Ag,0.,0.,1.829050381 Ag,1.7507342177,0.,-1.2233459218

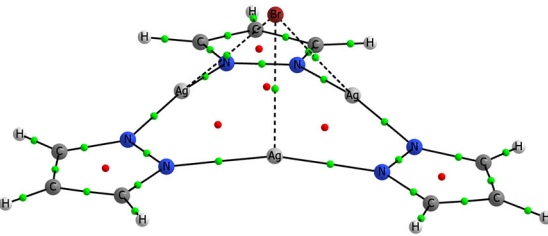
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	MP2= -1214.11580417 NIMAG= 0
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	N,0.6862934234,0.,-11.0536548133
	N,-2.7227886354,0.,-7.5330468534
	N,-2.0413937235,0.,-6.3472561119
	N,2.0413937235,0.,-6.3472561119
	N,2.7227886354,0.,-7.5330468534
	C,-1.1004084604,0.,-12.3648142217
	C,1.1004084604,0.,-12.3648142217
	C,-4.0593208349,0.,-7.255584776
	C,-2.950887713,0.,-5.3265221376
	C,2.950887713,0.,-5.3265221376
	C,4.0593208349,0.,-7.255584776
	C,0.,0.,-13.2433493619
	C,-4.2505103053,0.,-5.8617984367
	C,4.2505103053,0.,-5.8617984367
	H,-2.169220503,0.,-12.5841318783
	H,2.169220503,0.,-12.5841318783
	H,-4.7838428552,0.,-8.0693241122
	H,-2.6108541603,0.,-4.2912872004
	H,2.6108541603,0.,-4.2912872004
	H,4.7838428552,0.,-8.0693241122
	H,0.,0.,-14.394599871
	H,-5.1945262767,0.,-5.3190206376
	H,5.1945262767,0.,-5.3190206376
	Ag,-1.7090763326,0.,-9.3135118754
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	Ag,1.7090763326,0.,-9.3135118754
	F,0.,0.,-15.9481424453

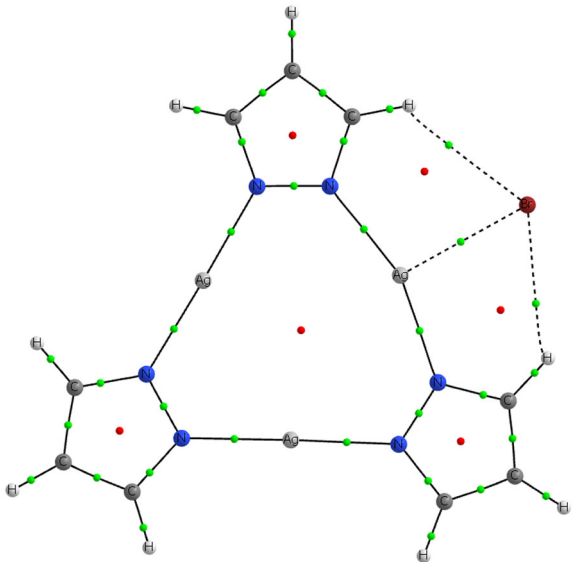
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	N,-
	0.6839155829,2.8001290572,0.0240455591
	N,2.7669445954,-
	0.8077740859,0.0240258614
	N,2.0830253936,-
	1.9923527544,0.0240288953
	N,-2.0830263646,-
	1.9923553868,0.0240354405

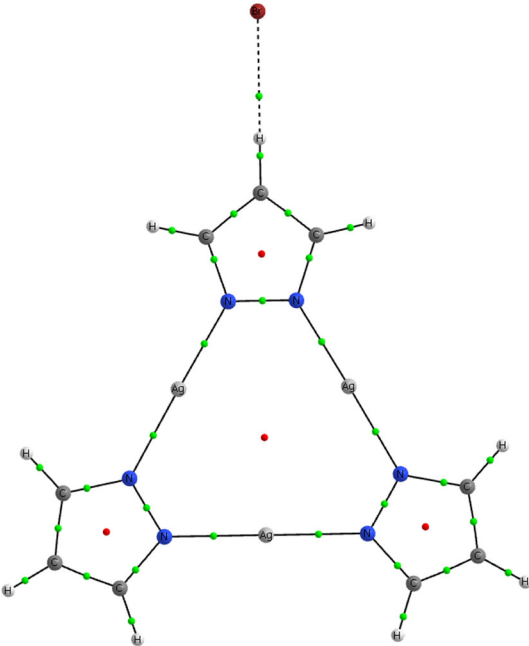
	N,-2.7669430716,- 0.8077767967,0.0240417649 C,1.1114686414,4.0885396839,0.173552390 4 C,- 1.1114679643,4.088544489,0.1734789895 C,4.0965181585,- 1.0817127979,0.173482467 C,2.9850439317,- 3.0068290795,0.1735142785 C,-2.9850443511,- 3.0068303836,0.1735323119 C,-4.0965174147,- 1.0817135881,0.1734950531 C,- 0.0000008222,4.9483007653,0.2695626533 C,4.2853527451,- 2.4741510912,0.2695501305 C,-4.2853540377,- 2.4741520727,0.2695570768 H,2.1788241702,4.3085496242,0.199686012 6 H,- 2.1788240978,4.308559391,0.1995435204 H,4.8207354565,- 0.2673638349,0.1995632093 H,2.6418994988,- 4.0411913281,0.1996256249 H,-2.6418998475,- 4.0411923126,0.1996488928 H,-4.8207336259,- 0.267363669,0.199576549 H,- 0.0000020685,6.0318760785,0.3868884585 H,5.223755621,- 3.0159401418,0.3868761316 H,-5.2237577836,- 3.0159405623,0.3868794658 Ag,1.6550622361,0.9555522823,- 0.1978392707 Ag,-0.0000010233,-1.9110913519,- 0.1978272832
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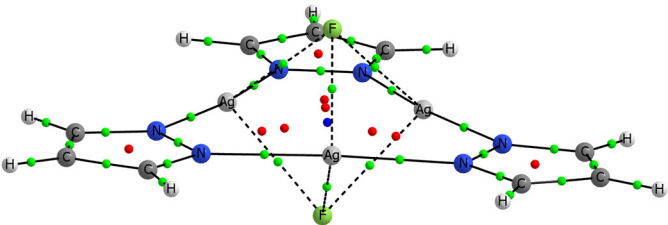
	<p>Ag,-1.6550545057,0.9555442535,-0.1978173302</p> <p>Cl,-0.0000071331,0.0000019217,-2.1860826093</p>
	<p>MP2= -1574.18904016 NIMAG= 0</p> <p>N,-0.6833251219,0,-2.9692456622</p> <p>N,0.6833251219,0,-2.9692456622</p> <p>N,-2.7638998472,0,0.5359922855</p> <p>N,-2.0872335055,0,1.7258839995</p> <p>N,2.0872335055,0,1.7258839995</p> <p>N,2.7638998472,0,0.5359922855</p> <p>C,-1.112178376,0,-4.2662456945</p> <p>C,1.112178376,0,-4.2662456945</p> <p>C,-4.1088191725,0,0.7959001435</p> <p>C,-3.0050224915,0,2.7344188175</p> <p>C,3.0050224915,0,2.7344188175</p> <p>C,4.1088191725,0,0.7959001435</p> <p>C,0,0,-5.1275182469</p> <p>C,-4.3044372289,0,2.1885259553</p> <p>C,4.3044372289,0,2.1885259553</p> <p>H,-2.1791341243,0,-4.4873262999</p> <p>H,2.1791341243,0,-4.4873262999</p> <p>H,-4.8267648508,0,-0.0250595036</p> <p>H,-2.6444070248,0,3.7643505735</p> <p>H,2.6444070248,0,3.7643505735</p> <p>H,4.8267648508,0,-0.0250595036</p> <p>H,0,0,-6.2166286351</p> <p>H,-5.2528205387,0,2.7250549727</p> <p>H,5.2528205387,0,2.7250549727</p> <p>Ag,-1.7113395525,0,-1.1978890657</p> <p>Ag,0,0,2.0318295468</p> <p>Ag,1.7113395525,0,-1.1978890657</p> <p>Cl,0,0,4.6543487698</p>

	<p>MP2= -1574.15919944 NIMAG= 0</p> <p>N,-0.6856840736,0,-11.0328638744</p> <p>N,0.6856840736,0,-11.0328638744</p> <p>N,-2.7225595204,0,-7.5087480286</p> <p>N,-2.0408672471,0,-6.3229482327</p> <p>N,2.0408672471,0,-6.3229482327</p> <p>N,2.7225595204,0,-7.5087480286</p> <p>C,-1.1064446174,0,-12.3381959093</p> <p>C,1.1064446174,0,-12.3381959093</p> <p>C,-4.0594712743,0,-7.2318026651</p> <p>C,-2.9508274138,0,-5.302840778</p> <p>C,2.9508274138,0,-5.302840778</p> <p>C,4.0594712743,0,-7.2318026651</p> <p>C,0,0,-13.2039544404</p> <p>C,-4.2502519215,0,-5.8383534486</p> <p>C,4.2502519215,0,-5.8383534486</p> <p>H,-2.1724918723,0,-12.5653311538</p> <p>H,2.1724918723,0,-12.5653311538</p> <p>H,-4.7841969491,0,-8.0453467611</p> <p>H,-2.6113232884,0,-4.2674717821</p> <p>H,2.6113232884,0,-4.2674717821</p> <p>H,4.7841969491,0,-8.0453467611</p> <p>H,0,0,-14.3051284283</p> <p>H,-5.1942445204,0,-5.2956972788</p> <p>H,5.1942445204,0,-5.2956972788</p> <p>Ag,-1.7113574517,0,-9.2879941689</p> <p>Ag,0,0,-6.3260491668</p> <p>Ag,1.7113574517,0,-9.2879941689</p> <p>Cl,0,0,-16.6715963889</p>
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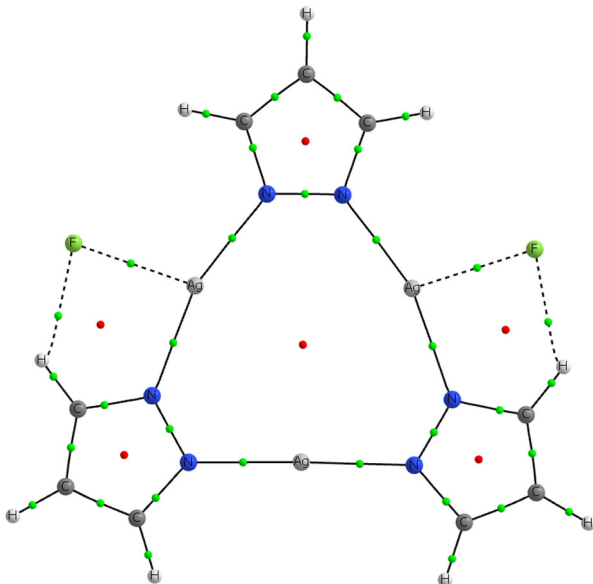
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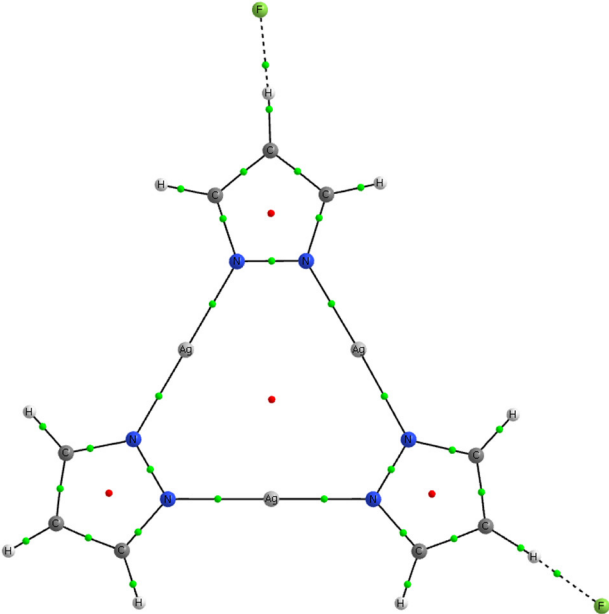
	C,0.0000008919,0.1989460471,4.9444537249 C,4.2820231192,0.198951225,-2.47222652 C,-4.2820225653,0.1989507437,-2.4722269151 H,2.1789512697,0.1204163544,4.3059167202 H,-2.1789506144,0.1204079026,4.3059215127 H,4.8185069626,0.1204474483,-0.2659300283 H,2.6395643335,0.1203887801,-4.039988815 H,-2.6395612287,0.1204015176,-4.0399869204 H,-4.8185089623,0.1204396003,-0.2659314376 H,0.0000019028,0.3300717882,6.0264628105 H,5.2190706387,0.3300775574,-3.0132305794 H,-5.219069767,0.3300760113,-3.0132318126 Ag,1.6486505574,-0.3206982665,0.9518486223 Ag,0.0000001653,-0.3206936447,-1.9036994699 Ag,-1.6486539607,-0.3206968676,0.9518502211 Br,-0.0000011215,-2.4502870355,-0.0000021695
	MP2= -1530.17909977 NIMAG= 0 N,-0.6832654207,0,-2.972035821 N,0.6832654207,0,-2.972035821 N,-2.7479078067,0,0.5396675271 N,-2.0920254668,0,1.7414005827 N,2.0920254668,0,1.7414005827 N,2.7479078067,0,0.5396675271 C,-1.1123713467,0,-4.2688724104 C,1.1123713467,0,-4.2688724104 C,-4.0975947407,0,0.7745819789 C,-3.0300705368,0,2.7316974133 C,3.0300705368,0,2.7316974133 C,4.0975947407,0,0.7745819789 C,0,0,-5.1299365448 C,-4.3192635575,0,2.1628392081 C,4.3192635575,0,2.1628392081 H,-2.1792972672,0,-4.4900212035 H,2.1792972672,0,-4.4900212035 H,-4.7999855152,0,-0.0597674736 H,-2.6934849008,0,3.7693379561 H,2.6934849008,0,3.7693379561 H,4.7999855152,0,-0.0597674736 H,0,0,-6.2190360851 H,-5.2770275092,0,2.682338107 H,5.2770275092,0,2.682338107 Ag,-1.6990965176,0,-1.1947430262 Ag,0,0,2.0923742588

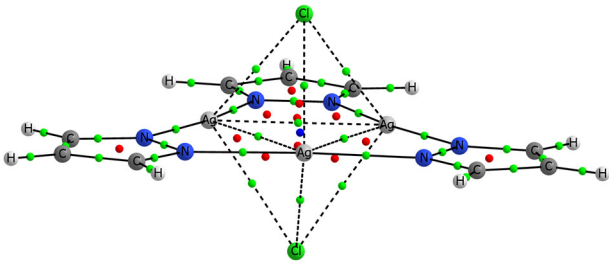
	Ag,1.6990965176,0,-1.1947430262 Br,0,0,4.8145051728
	MP2= -1530.14938477 NIMAG= 0 N,-0.6856232851,0,-11.0269202899 N,0.6856232851,0,-11.0269202899 N,-2.7225435465,0,-7.5023755717 N,-2.0408323992,0,-6.3165210514 N,2.0408323992,0,-6.3165210514 N,2.7225435465,0,-7.5023755717 C,-1.1071291941,0,-12.3314858688 C,1.1071291941,0,-12.3314858688 C,-4.0595196231,0,-7.2255166244 C,-2.9508719393,0,-5.2965539889 C,2.9508719393,0,-5.2965539889 C,4.0595196231,0,-7.2255166244 C,0,0,-13.1958470574 C,-4.2502648684,0,-5.8321289678 C,4.2502648684,0,-5.8321289678 H,-2.1729415999,0,-12.5592955383 H,2.1729415999,0,-12.5592955383 H,-4.7843038795,0,-8.0390117519 H,-2.6114527296,0,-4.2611650215 H,2.6114527296,0,-4.2611650215 H,4.7843038795,0,-8.0390117519 H,0,0,-14.2938450907 H,-5.1942538977,0,-5.2894915585 H,5.1942538977,0,-5.2894915585 Ag,-1.71166461,0,-9.2813016475 Ag,0,0,-6.3192655303 Ag,1.71166461,0,-9.2813016475 Br,0,0,-16.8494231353

	MP2= -1313.77137985 NIMAG= 0 X X,1,r21 X,1,r21,2,120. X,1,r21,2,120.,3,180.,0 N,2,r52,1,90.,3,0.,0 N,2,r52,1,90.,4,0.,0 N,3,r52,1,90.,2,0.,0 N,3,r52,1,90.,4,0.,0 N,4,r52,1,90.,3,0.,0
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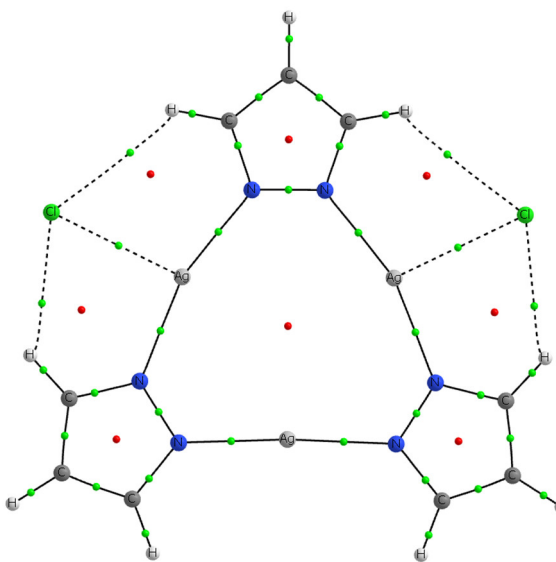
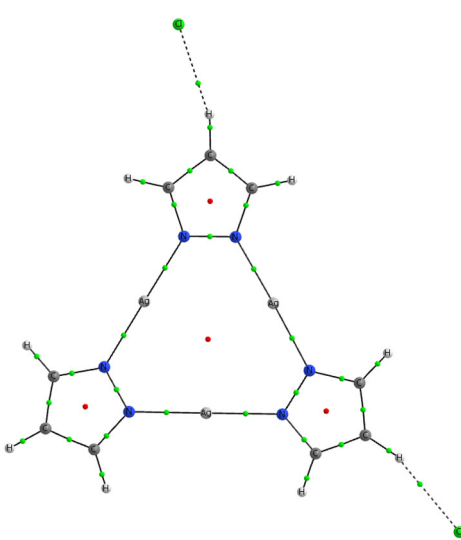
	N,4,r52,1,90.,2,0.,0 C,5,r115,2,a1152,1,180.,0 C,6,r115,2,a1152,1,180.,0 C,7,r115,3,a1152,1,180.,0 C,8,r115,3,a1152,1,180.,0 C,9,r115,4,a1152,1,180.,0 C,10,r115,4,a1152,1,180.,0 C,1,r171,3,120.,2,0.,0 C,1,r171,4,120.,3,0.,0 C,1,r171,2,120.,4,0.,0 H,11,r2011,5,a20115,2,180.,0 H,12,r2011,6,a20115,2,180.,0 H,13,r2011,7,a20115,3,180.,0 H,14,r2011,8,a20115,3,180.,0 H,15,r2011,9,a20115,4,180.,0 H,16,r2011,10,a20115,4,180.,0 H,1,r261,3,120.,2,0.,0 H,1,r261,4,120.,3,0.,0 H,1,r261,2,120.,4,0.,0 Ag,1,r291,3,60.,2,0.,0 Ag,1,r291,4,60.,3,0.,0 Ag,1,r291,2,60.,4,0.,0 F,1,rcl,2,90.,3,90.,0 F,1,rcl,2,90.,3,-90.,0 r21=2.87160594 r52=0.68467026 r115=1.36549193 r171=5.04193545 r2011=1.09128504 r261=6.13395387 r291=1.85382051 a1152=108.16910165 a20115=119.80782174 rcl=1.58245635
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	N,0.6340192821,0.,2.7693317219
	N,-0.7337615116,0.,2.7813064002
	N,2.7849830503,0.,-0.816363517
	N,2.0994830696,0.,-2.0036843122
	N,-2.0813019816,0.,-1.9337426657
	N,-2.7755627541,0.,-0.7551970908
	C,1.0799539837,0.,4.0569536436
	C,-1.155372962,0.,4.0851811306
	C,4.123013411,0.,-1.0936246373
	C,3.0086134236,0.,-3.0238220354
	C,-2.9734479254,0.,-2.9637444066
	C,-4.1155571191,0.,-1.0420082294
	C,-0.0285365756,0.,4.9322596728
	C,4.3150572906,0.,-2.4912994883
	C,-4.2857304625,0.,-2.4414164371
	H,2.1655580465,0.,4.1976493486
	H,-2.2219152569,0.,4.3163401187
	H,4.8325014489,0.,-0.2642845155
	H,2.6451278287,0.,-4.0529267608
	H,-2.5524919488,0.,-3.974252956
	H,-4.8490178227,0.,-0.2339350018
	H,-0.0210822566,0.,6.0232208091
	H,5.2600272911,0.,-3.0368781725
	H,-5.2268033616,0.,-2.9933526347
	Ag,1.9808205748,0.,1.1228144764
	Ag,0.0180244271,0.,-2.2768481764
	Ag,-1.7284735485,0.,0.9979346685
	F,3.7186453294,0.,2.6696607397
	F,-0.4526713554,0.,-4.5552716928

	MP2= -1313.76077782 NIMAG= 0 N,0.6834719946,0.,2.706992012 N,-0.6834719946,0.,2.706992012 N,2.7117133194,0.,-0.8226119284 N,2.0369437493,0.,-2.0167850507 N,-2.0369437493,0.,-2.0167850507 N,-2.7117133194,0.,-0.8226119284 C,1.1125748895,0.,4.0036159513 C,-1.1125748895,0.,4.0036159513 C,4.0581026893,0.,-1.0997043486 C,2.9770234624,0.,-3.0187282969 C,-2.9770234624,0.,-3.0187282969 C,-4.0581026893,0.,-1.0997043486 C,0.,0.,4.8652668149 C,4.2836377419,0.,-2.4888538381 C,-4.2836377419,0.,-2.4888538381 H,2.1798587122,0.,4.2235837635 H,-2.1798587122,0.,4.2235837635 H,4.7739184331,0.,-0.2763690913 H,2.6434227894,0.,-4.0573978808 H,-2.6434227894,0.,-4.0573978808 H,-4.7739184331,0.,-0.2763690913 H,0.,0.,5.9545732176 H,5.2843267048,0.,-3.0222652324 H,-5.2843267048,0.,-3.0222652324 Ag,1.7007952942,0.,0.9270998121 Ag,0.,0.,-2.0434036517 Ag,-1.7007952942,0.,0.9270998121 F,6.8010654903,0.,-3.6967940582 F,-6.8010654903,0.,-3.6967940582
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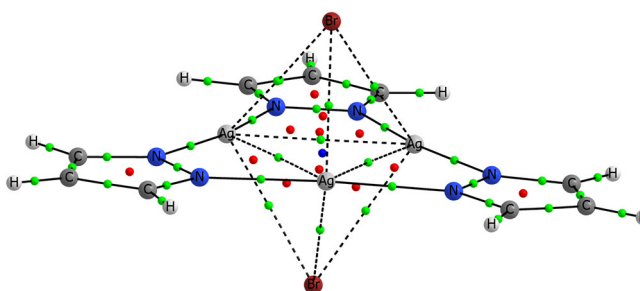
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	C,5,r115,2,a1152,1,180.,0
	C,6,r115,2,a1152,1,180.,0
	C,7,r115,3,a1152,1,180.,0
	C,8,r115,3,a1152,1,180.,0
	C,9,r115,4,a1152,1,180.,0
	C,10,r115,4,a1152,1,180.,0
	C,1,r171,3,120.,2,0.,0
	C,1,r171,4,120.,3,0.,0
	C,1,r171,2,120.,4,0.,0
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	H,12,r2011,6,a20115,2,180.,0
	H,13,r2011,7,a20115,3,180.,0
	H,14,r2011,8,a20115,3,180.,0
	H,15,r2011,9,a20115,4,180.,0
	H,16,r2011,10,a20115,4,180.,0
	H,1,r261,3,120.,2,0.,0
	H,1,r261,4,120.,3,0.,0
	H,1,r261,2,120.,4,0.,0
	Ag,1,r291,3,60.,2,0.,0
	Ag,1,r291,4,60.,3,0.,0
	Ag,1,r291,2,60.,4,0.,0
	Cl,1,rcl,2,90.,3,90.,0
	Cl,1,rcl,2,90.,3,-90.,0
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	r52=0.68373106
	r115=1.36520889
	r171=5.03777307
	r2011=1.09116016
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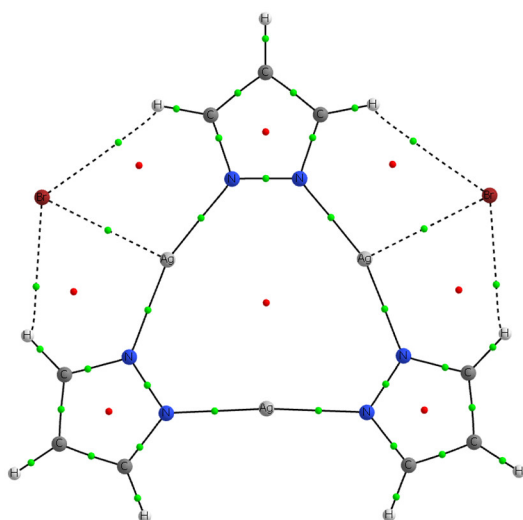
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	<p>MP2= -2033.85619152 NIMAG= 0</p> <p>N,0.6836020158,0.,2.6864675021</p> <p>N,-0.6836020158,0.,2.6864675021</p> <p>N,2.7130971773,0.,-0.8454242555</p> <p>N,2.0379369488,0.,-2.0384224112</p> <p>N,-2.0379369488,0.,-2.0384224112</p> <p>N,-2.7130971773,0.,-0.8454242555</p> <p>C,1.112651153,0.,3.9831782774</p> <p>C,-1.112651153,0.,3.9831782774</p> <p>C,4.0569240634,0.,-1.1156322219</p> <p>C,2.9696968284,0.,-3.0444022067</p> <p>C,-2.9696968284,0.,-3.0444022067</p> <p>C,-4.0569240634,0.,-1.1156322219</p>

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	C,4.2684960599,0,-2.5039480128
	C,-4.2684960599,0,-2.5039480128
	H,2.1797366064,0,4.2037702504
	H,-2.1797366064,0,4.2037702504
	H,4.7818462464,0,-0.301991067
	H,2.6390712975,0,-4.0830915091
	H,-2.6390712975,0,-4.0830915091
	H,-4.7818462464,0,-0.301991067
	H,0,0,5.9330474203
	H,5.2415901892,0,-3.0110219699
	H,-5.2415901892,0,-3.0110219699
	Ag,1.7037047019,0,0.9114268027
	Ag,0,0,-2.0634322486
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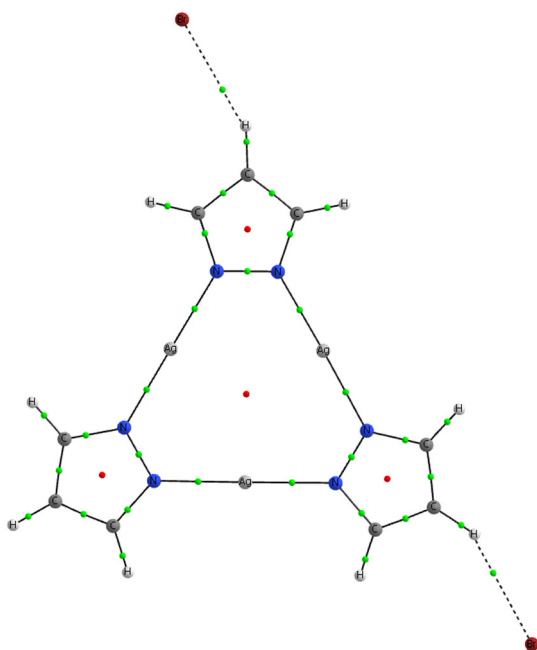
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	N,-
	0.6836387761,0.0000858494,2.869500323
	N,2.8268793284,0.0000837422,-
	0.8427016069
	N,2.1432406546,0.0000808228,-
	2.0268030038
	N,-2.143241689,0.0000802372,-
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	N,-2.8268805375,0.0000857215,-
	0.8427015024
	C,1.1110670304,-
	0.0000194003,4.1659217533
	C,-1.1110658242,-
	0.0000165907,4.1659191363
	C,4.1633246362,-0.0000199535,-
	1.1207476111
	C,3.0522610253,-0.0000185799,-
	3.0451732505
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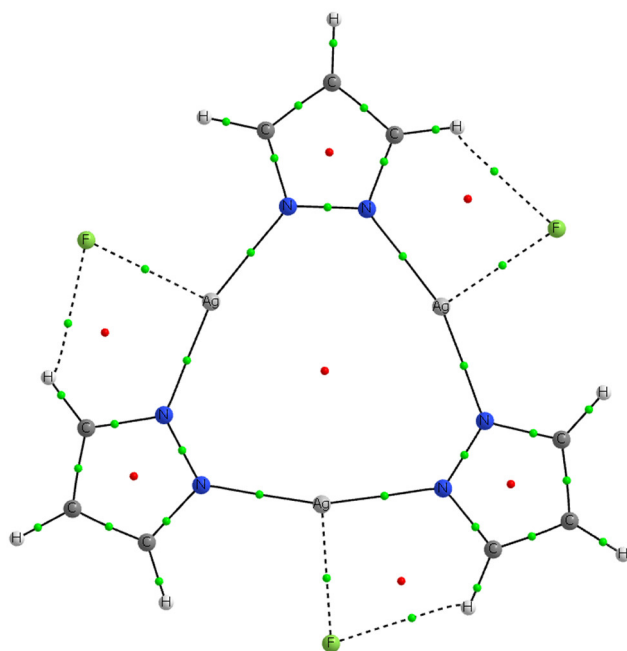
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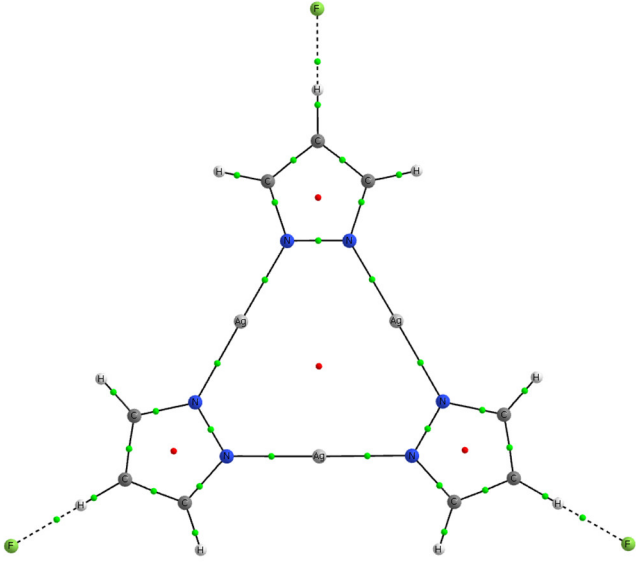
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 N,2.0638661479,0.,-1.9839139669
 N,-2.1090285212,0.,-1.999387489
 N,-2.7268945206,0.,-0.7787587814
 C,1.0301882945,0.,4.1433774874
 C,-1.1969830942,0.,4.0226829313
 C,4.0891032452,0.,-1.0728660453
 C,2.9736808727,0.,-3.0048342664
 C,-3.0731760144,0.,-2.9638579774
 C,-4.082237157,0.,-0.9747236982
 C,-0.1315191742,0.,4.9428907954
 C,4.2768110622,0.,-2.469218018
 C,-4.3464285841,0.,-2.3575464518
 H,2.0913615726,0.,4.3966365256
 H,-2.2764225464,0.,4.1807053333
 H,4.7985993818,0.,-0.243754698
 H,2.6103974517,0.,-4.0338316182
 H,-2.7619181361,0.,-4.0094905132
 H,-4.7588082976,0.,-0.1189129118
 H,-0.1926751989,0.,6.0314838369
 H,5.2213702236,0.,-3.0145595041
 H,-5.3197558247,0.,-2.8488803016
 Ag,1.9929156,0.,1.1618628371
 Ag,-0.0097449327,0.,-2.3068469558
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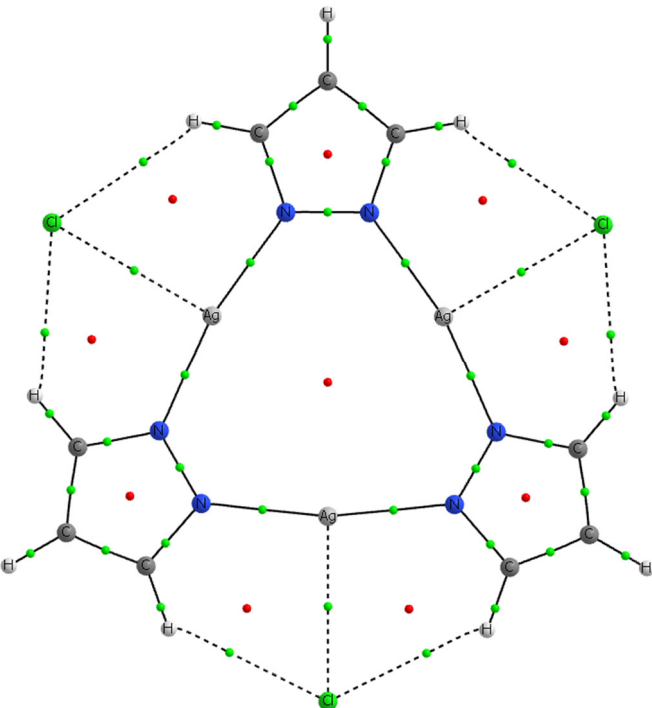
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 N,2.0372711729,0.,-2.071068092
 N,-2.0372711729,0.,-2.071068092
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 C,4.0593644215,0.,-1.1535418219
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 C,-2.9643604894,0.,-3.0809387432
 C,-4.0593644215,0.,-1.1535418219
 C,0.,0.,4.8077176394
 C,4.2633378613,0.,-2.5424596029
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 H,2.1797534587,0.,4.1678867218
 H,-2.1797534587,0.,4.1678867218
 H,4.7919299349,0.,-0.3469880165
 H,2.629407205,0.,-4.1182201216
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 H,0.,0.,5.8967947659
 H,5.2356565499,0.,-3.0433772421
 H,-5.2356565499,0.,-3.0433772421
 Ag,1.7076887209,0.,0.8780474971
 Ag,0.,0.,-2.092108668
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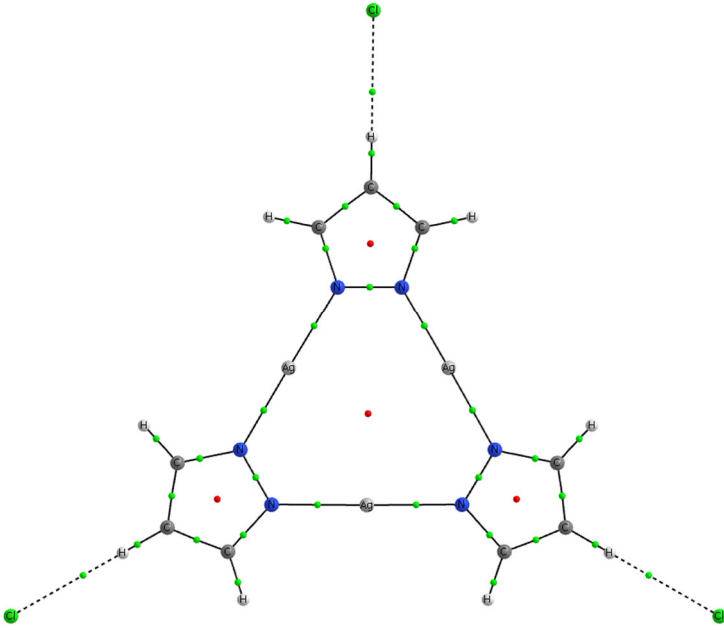


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 N,-2.7766291359,0.7955427971,0.
 N,-0.6717914492,-2.8312640559,0.
 N,0.6990362856,-2.802046163,0.
 C,2.9567938161,3.0509702582,0.
 C,4.1193772809,1.1409895713,0.
 C,-3.0475670163,2.997120365,0.
 C,-4.1210150428,1.035593887,0.
 C,-1.0716693873,-4.1380015281,0.
 C,1.1637496209,-4.0861920796,0.
 C,4.2774018335,2.5458760107,0.
 C,-4.3434058262,2.4318904064,0.
 C,0.0659988538,-4.9772860986,0.
 H,2.5400814212,4.0618687343,0.
 H,4.8424027577,0.3223866829,0.
 H,-2.6997122779,4.0324017526,0.
 H,-4.7881785659,0.1693542652,0.
 H,-2.1420618506,-4.3550362123,0.
 H,2.2475968949,-4.2304810244,0.
 H,5.2114791522,3.1129020416,0.
 H,-5.301392823,2.9576608309,0.
 H,0.0897529614,-6.0697788229,0.
 Ag,-0.0230337063,2.3036672882,0.
 Ag,-1.9844364922,-1.172171348,0.
 Ag,2.0068671051,-1.1321019238,0.
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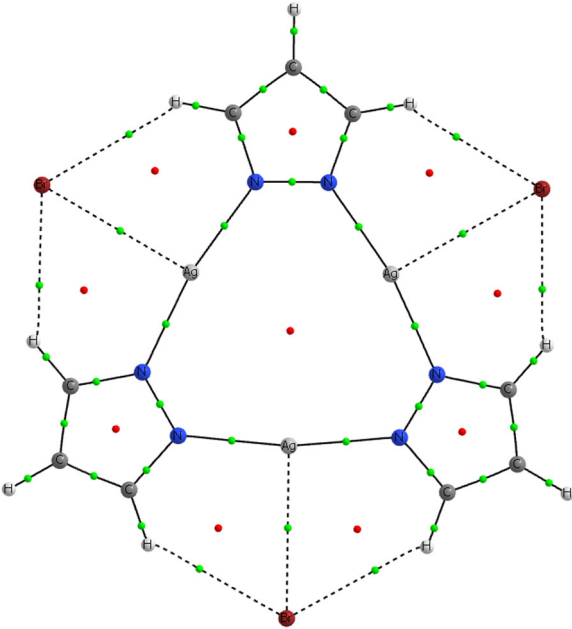
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	a1152=107.65730918 a20115=119.23117844 rf=7.83637357
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	MP2= -2493.49098353 NIMAG= 0 X X,1,r21 X,1,r21,2,120. X,1,r21,2,120.,3,180.,0 N,2,r52,1,90.,3,0.,0 N,2,r52,1,90.,4,0.,0 N,3,r52,1,90.,2,0.,0 N,3,r52,1,90.,4,0.,0 N,4,r52,1,90.,3,0.,0 N,4,r52,1,90.,2,0.,0 C,5,r115,2,a1152,1,180.,0 C,6,r115,2,a1152,1,180.,0 C,7,r115,3,a1152,1,180.,0 C,8,r115,3,a1152,1,180.,0 C,9,r115,4,a1152,1,180.,0 C,10,r115,4,a1152,1,180.,0 C,1,r171,3,120.,2,0.,0 C,1,r171,4,120.,3,0.,0 C,1,r171,2,120.,4,0.,0 H,11,r2011,5,a20115,2,180.,0 H,12,r2011,6,a20115,2,180.,0 H,13,r2011,7,a20115,3,180.,0 H,14,r2011,8,a20115,3,180.,0 H,15,r2011,9,a20115,4,180.,0 H,16,r2011,10,a20115,4,180.,0 H,1,r261,3,120.,2,0.,0 H,1,r261,4,120.,3,0.,0 H,1,r261,2,120.,4,0.,0 Ag,1,r291,3,60.,2,0.,0 Ag,1,r291,4,60.,3,0.,0 Ag,1,r291,2,60.,4,0.,0 Cl,1,rf,3,60.,2,0.,0 Cl,1,rf,4,60.,3,0.,0 Cl,1,rf,2,60.,4,0.,0 r21=2.79397013 r52=0.68571669
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	r115=1.36612675 r171=4.95001333 r2011=1.09202493 r261=6.04151947 r291=2.19264029 a1152=108.47621532 a20115=118.51123295 rf=5.21805156
	MP2= -2493.51272106 NIMAG=0 N,0.6851598509,0.,2.7501859923 N,-0.6851598509,0.,2.7501859923 N,2.7243117377,0.,-0.781722259 N,2.0391442088,0.,-1.968445031 N,-2.0391442088,0.,-1.968445031 N,-2.7243117377,0.,-0.781722259 C,1.1072561745,0.,4.0540494066 C,-1.1072561745,0.,4.0540494066 C,4.0645351664,0.,-1.0681191336 C,2.9572600363,0.,-2.9859358616 C,-2.9572600363,0.,-2.9859358616 C,-4.0645351664,0.,-1.0681191336 C,0.,0.,4.9215300289 C,4.2621530781,0.,-2.460775003 C,-4.2621530781,0.,-2.460775003 H,2.1738111543,0.,4.2785608512 H,-2.1738111543,0.,4.2785608512 H,4.7922521737,0.,-0.2567172315 H,2.6184028184,0.,-4.0218514866 H,-2.6184028184,0.,-4.0218514866 H,-4.7922521737,0.,-0.2567172315 H,0.,0.,6.0179285632 H,5.2116562812,0.,-3.0089840097 H,-5.2116562812,0.,-3.0089840097 Ag,1.7123650959,0.,0.9886341926 Ag,0.,0.,-1.977205477

	Ag,- 1.7123650959,0.,0.9886341926 Cl,7.584478187,0.,-4.3789157976 Cl,-7.584478187,0.,-4.3789157976 Cl,0.,0.,8.7578186132
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	MP2= -2361.46823649 NIMAG= 0 X X,1,r21 X,1,r21,2,120. X,1,r21,2,120.,3,180.,0 N,2,r52,1,90.,3,0.,0 N,2,r52,1,90.,4,0.,0 N,3,r52,1,90.,2,0.,0 N,3,r52,1,90.,4,0.,0 N,4,r52,1,90.,3,0.,0 N,4,r52,1,90.,2,0.,0 C,5,r115,2,a1152,1,180.,0 C,6,r115,2,a1152,1,180.,0 C,7,r115,3,a1152,1,180.,0 C,8,r115,3,a1152,1,180.,0 C,9,r115,4,a1152,1,180.,0 C,10,r115,4,a1152,1,180.,0 C,1,r171,3,120.,2,0.,0 C,1,r171,4,120.,3,0.,0 C,1,r171,2,120.,4,0.,0 H,11,r2011,5,a20115,2,180.,0 H,12,r2011,6,a20115,2,180.,0 H,13,r2011,7,a20115,3,180.,0 H,14,r2011,8,a20115,3,180.,0 H,15,r2011,9,a20115,4,180.,0 H,16,r2011,10,a20115,4,180.,0 H,1,r261,3,120.,2,0.,0 H,1,r261,4,120.,3,0.,0 H,1,r261,2,120.,4,0.,0 Ag,1,r291,3,60.,2,0.,0 Ag,1,r291,4,60.,3,0.,0 Ag,1,r291,2,60.,4,0.,0 Br,1,rf,3,60.,2,0.,0 Br,1,rf,4,60.,3,0.,0 Br,1,rf,2,60.,4,0.,0 r21=2.78777393
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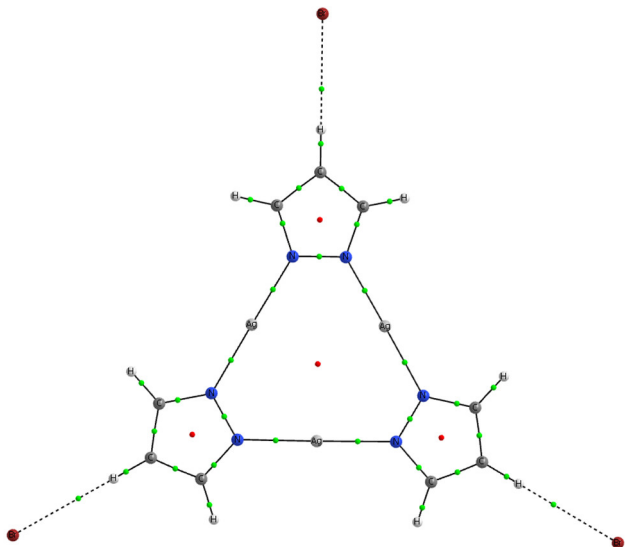
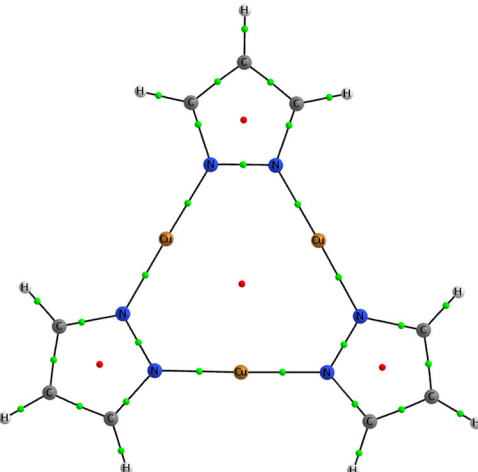
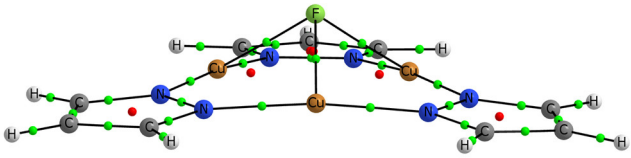
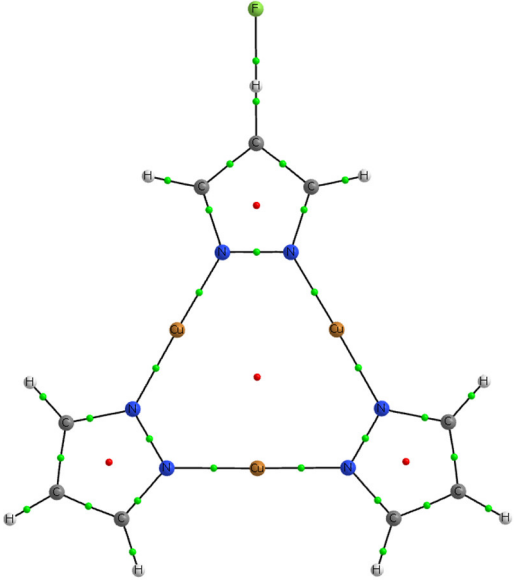
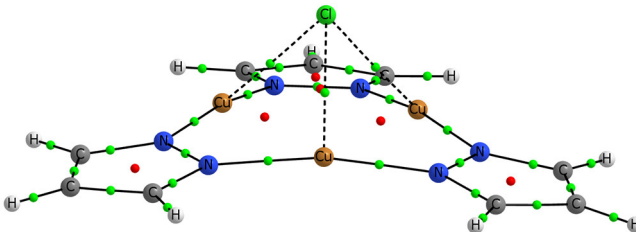
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	MP2= -2361.48741177 NIMAG= 0 N,0.6850495639,0.,2.7503041832 N,-0.6850495639,0.,2.7503041832 N,2.7243518812,0.,-0.7818772151 N,2.0393017978,0.,-1.9684153026 N,-2.0393017978,0.,-1.9684153026 N,-2.7243518812,0.,-0.7818772151 C,1.1079138977,0.,4.0534702125 C,-1.1079138977,0.,4.0534702125 C,4.0643589206,0.,-1.0672503843 C,2.9564411232,0.,-2.9862122949 C,-2.9564411232,0.,-2.9862122949 C,-4.0643589206,0.,-1.0672503843 C,0.,0.,4.9196369031 C,4.26052172,0.,-2.459816028 C,-4.26052172,0.,-2.459816028 H,2.1742791756,0.,4.2784256277 H,-2.1742791756,0.,4.2784256277 H,4.7923598312,0.,-0.2562296466 H,2.6180733793,0.,-4.0221887626 H,-2.6180733793,0.,-4.0221887626 H,-4.7923598312,0.,-0.2562296466 H,0.,0.,6.0143474095 H,5.2085675349,0.,-3.0071732989 H,-5.2085675349,0.,-3.0071732989 Ag,1.7127257571,0.,0.9888475796 Ag,0.,0.,-1.9776712736 Ag,-1.7127257571,0.,0.9888475796 Br,7.779709616,0.,-4.4916761175 Br,-7.779709616,0.,-4.4916761175 Br,0.,0.,8.9832708121

Table S3. Molecular graph, electronic energy and geometry of the (Pz-Cu)₃:X⁻ⁿ complexes.

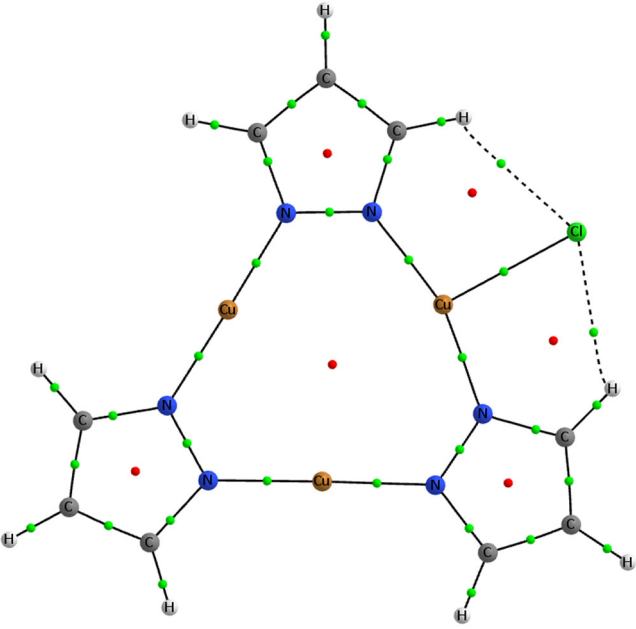
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	N,2,r52,1,90.,4,0.,0
	N,3,r52,1,90.,2,0.,0
	N,3,r52,1,90.,4,0.,0
	N,4,r52,1,90.,3,0.,0
	N,4,r52,1,90.,2,0.,0
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	C,6,r115,2,a1152,1,180.,0
	C,7,r115,3,a1152,1,180.,0
	C,8,r115,3,a1152,1,180.,0
	C,9,r115,4,a1152,1,180.,0
	C,10,r115,4,a1152,1,180.,0
	C,1,r171,3,120.,2,0.,0
	C,1,r171,4,120.,3,0.,0
	C,1,r171,2,120.,4,0.,0
	H,11,r2011,5,a20115,2,180.,0
	H,12,r2011,6,a20115,2,180.,0
	H,13,r2011,7,a20115,3,180.,0
	H,14,r2011,8,a20115,3,180.,0
	H,15,r2011,9,a20115,4,180.,0
	H,16,r2011,10,a20115,4,180.,0
	H,1,r261,3,120.,2,0.,0
	H,1,r261,4,120.,3,0.,0
	H,1,r261,2,120.,4,0.,0
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	Cu,1,r291,4,60.,3,0.,0
	Cu,1,r291,2,60.,4,0.,0
	r21=2.49391542
	r52=0.68517656
	r115=1.36634178
	r171=4.64884563
	r2011=1.08892227
	r261=5.73710754
	r291=1.85459423
	a1152=108.21748163
	a20115=120.11537875

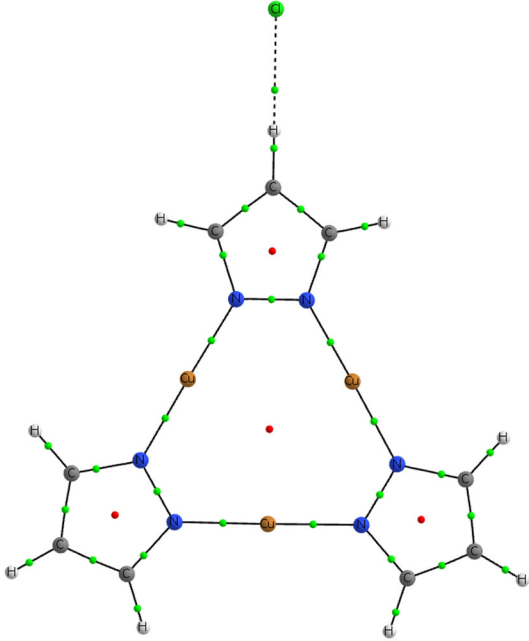
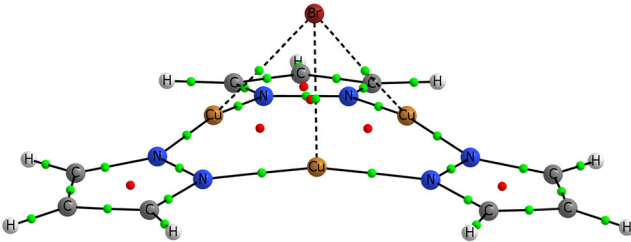
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	0.6870979556,2.5189761251,0.0162613917
	N,2.5249251179,-
	0.6644761179,0.0162611276
	N,1.8379307704,-
	1.8544851676,0.0162503429
	N,-1.8379506548,-
	1.8544124181,0.016244903
	N,-2.52503866,-0.6644688411,0.0162354006
	C,1.1112828867,3.8119968856,0.123550136
	8
	C,-
	1.1111932548,3.8121479414,0.1235451682
	C,3.8569335789,-0.943640824,0.1234868565
	C,2.745763744,-2.8683944107,0.1234699896
	C,-2.7457029753,-
	2.8683995782,0.1234366781
	C,-3.8570335117,-
	0.9437281407,0.1234249828
	C,0.0001070475,4.6736328286,0.187985139
	5
	C,4.0474872087,-2.336767153,0.1880844424
	C,-4.0474662678,-
	2.3368657435,0.1881454783
	H,2.1778568194,4.0302603416,0.149487298
	2
	H,-
	2.1777389769,4.0305464578,0.1494779514
	H,4.5792678287,-
	0.1291147408,0.1493971196
	H,2.4015980576,-
	3.9012402285,0.1493621317
	H,-2.4014471189,-
	3.901212967,0.1493089606
	H,-4.5794390187,-
	0.1292627477,0.1492876056
	H,0.0001809541,5.7601237179,0.270572407
	8
	H,4.9884313658,-
	2.8799707239,0.2707702184

	<p>H,-4.9883612942,- 2.8801457192,0.2708904207 Cu,1.5696330879,0.906253833,- 0.102368143 Cu,-0.0000129908,-1.8125702477,- 0.1024046546 Cu,-1.5698380526,0.9063165117,- 0.1023856193 F,-0.0000628182,0.0000214356,- 1.2313911312</p>
	<p>MP2= -1365.04081154 NIMAG= 0 N,-0.6843596385,0,-2.6945780783 N,0.6843596385,0,-2.6945780783 N,-2.5563172697,0,0.4248884925 N,-1.8303680365,0,1.586102275 N,1.8303680365,0,1.586102275 N,2.5563172697,0,0.4248884925 C,-1.1120075647,0,-3.9920762603 C,1.1120075647,0,-3.9920762603 C,-3.8877630448,0,0.7433775147 C,-2.7008930959,0,2.6353328471 C,2.7008930959,0,2.6353328471 C,3.8877630448,0,0.7433775147 C,0,0,-4.8525783728 C,-4.0213397566,0,2.1439512732 C,4.0213397566,0,2.1439512732 H,-2.1783817174,0,-4.2126404155 H,2.1783817174,0,-4.2126404155 H,-4.6403662067,0,-0.0451031743 H,-2.2741711033,0,3.6389095102 H,2.2741711033,0,3.6389095102 H,4.6403662067,0,-0.0451031743 H,0,0,-5.9415104408 H,-4.9466073638,0,2.7193073255 H,4.9466073638,0,2.7193073255 Cu,-1.6159896501,0,-1.1266289386 Cu,0,0,1.763661584 Cu,1.6159896501,0,-1.1266289386 F,0,0,3.7794949636</p>

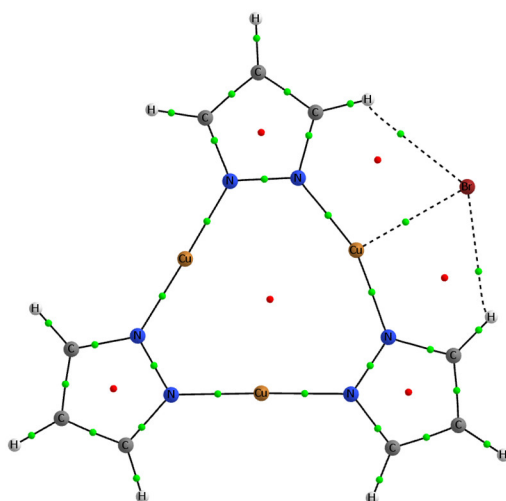
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	<p>MP2= -1725.07834839 NIMAG= 0</p> <p>N,0.6855128138,2.5150704687,-0.0163992513</p> <p>N,-0.6855251099,2.5150421796,-0.0164166807</p> <p>N,2.5209067205,-0.6638627454,-0.0164221605</p> <p>N,1.8353617657,-1.851192956,-0.0163991263</p> <p>N,-1.8353481588,-1.8511667539,-0.0164009983</p> <p>N,-2.5208854105,-0.6638278683,-0.0164350464</p>

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	C,3.8461109931,-
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	C,-2.7343272514,-
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	Cu,1.5573106226,0.8990846545,-
	0.2020603201
	Cu,0.0000097313,-1.7981096418,-
	0.2020478598
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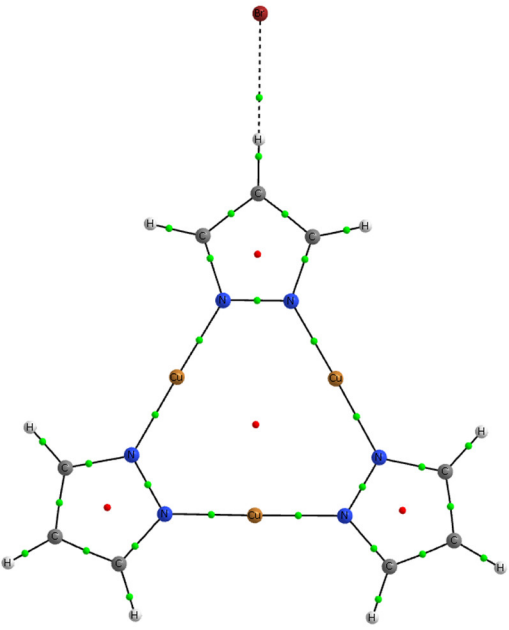
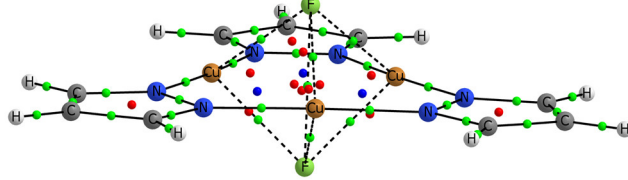
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	N,-1.8438486766,0,1.6587192415
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	N,2.4853905617,0,0.4457624952
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	C,1.1129627489,0,-4.0017992679
	C,-3.8381517048,0,0.6615803732
	C,-2.8003285729,0,2.6331216235
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	C,3.8381517048,0,0.6615803732
	C,0,0,-4.861249712
	C,-4.0790673725,0,2.0450727069
	C,4.0790673725,0,2.0450727069
	H,-2.1791978152,0,-4.2229894623
	H,2.1791978152,0,-4.2229894623
	H,-4.527112547,0,-0.1831869739
	H,-2.4776374526,0,3.6735267945
	H,2.4776374526,0,3.6735267945
	H,4.527112547,0,-0.1831869739
	H,0,0,-5.9500606632
	H,-5.0436216973,0,2.5513404874
	H,5.0436216973,0,2.5513404874
	Cu,-1.5688183432,0,-1.1140439207
	Cu,0,0,1.9442950537
	Cu,1.5688183432,0,-1.1140439207
	Cl,0,0,4.3740041705

	<p>MP2= -1725.04771008 NIMAG= 0</p> <p>N,-0.6870325399,0,-10.790425632</p> <p>N,0.6870325399,0,-10.790425632</p> <p>N,-2.4981865692,0,-7.6440384859</p> <p>N,-1.8178503724,0,-6.4551119499</p> <p>N,1.8178503724,0,-6.4551119499</p> <p>N,2.4981865692,0,-7.6440384859</p> <p>C,-1.1060969794,0,-12.0960771275</p> <p>C,1.1060969794,0,-12.0960771275</p> <p>C,-3.8353234421,0,-7.3692525211</p> <p>C,-2.7309738311,0,-5.4377094503</p> <p>C,2.7309738311,0,-5.4377094503</p> <p>C,3.8353234421,0,-7.3692525211</p> <p>C,0,0,-12.9609294259</p> <p>C,-4.0277667659,0,-5.9767406202</p> <p>C,4.0277667659,0,-5.9767406202</p> <p>H,-2.1713200717,0,-12.3246215867</p> <p>H,2.1713200717,0,-12.3246215867</p> <p>H,-4.55813137,0,-8.1837287593</p> <p>H,-2.394365026,0,-4.4020370526</p> <p>H,2.394365026,0,-4.4020370526</p> <p>H,4.55813137,0,-8.1837287593</p> <p>H,0,0,-14.0619893265</p> <p>H,-4.9726854107,0,-5.4364145387</p> <p>H,4.9726854107,0,-5.4364145387</p> <p>Cu,-1.6020043835,0,-9.2302271682</p> <p>Cu,0,0,-6.4470263381</p> <p>Cu,1.6020043835,0,-9.2302271682</p> <p>Cl,0,0,-16.4192017066</p>
	<p>MP2= -1681.06662494 NIMAG= 0</p> <p>N,0.6850400295,-</p> <p>0.1101182553,2.5133088822</p> <p>N,-0.6850889835,-</p> <p>0.1101440945,2.5133342746</p> <p>N,2.5191687567,-0.1101320505,-</p> <p>0.6633909732</p> <p>N,1.8341193884,-0.1101203042,-</p> <p>1.8499536979</p> <p>N,-1.8341003149,-0.1100912801,-</p> <p>1.8499527345</p> <p>N,-2.5191546542,-0.1101125597,-</p> <p>0.6633773526</p>

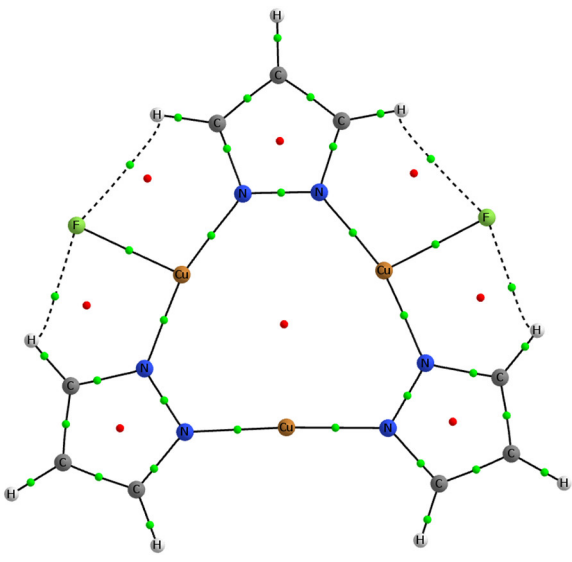
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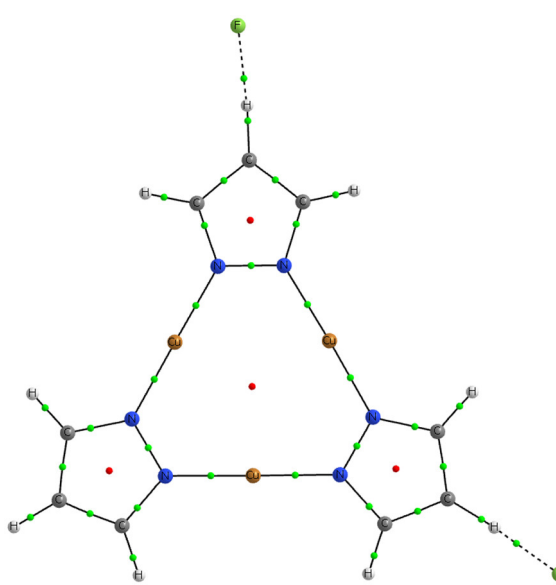


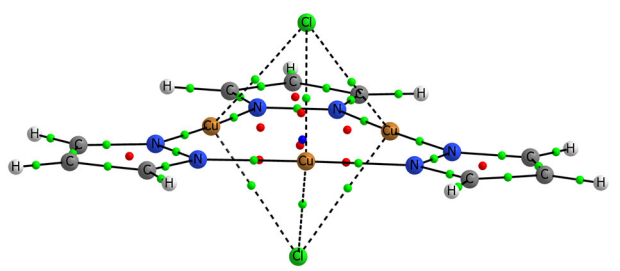
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 N,-1.8459707228,0,1.671739356
 N,1.8459707228,0,1.671739356
 N,2.4697199599,0,0.4487525566
 C,-1.113201974,0,-4.0054672217
 C,1.113201974,0,-4.0054672217
 C,-3.8257128408,0,0.6438020175
 C,-2.8190847386,0,2.6300074155
 C,2.8190847386,0,2.6300074155
 C,3.8257128408,0,0.6438020175
 C,0,0,-4.86466821
 C,-4.0883477706,0,2.0227594208
 C,4.0883477706,0,2.0227594208
 H,-2.1794123351,0,-4.226719722
 H,2.1794123351,0,-4.226719722
 H,-4.5011673301,0,-0.2118372021
 H,-2.5185260383,0,3.6766480173
 H,2.5185260383,0,3.6766480173
 H,4.5011673301,0,-0.2118372021
 H,0,0,-5.9534556105
 H,-5.0600874531,0,2.5148664302
 H,5.0600874531,0,2.5148664302
 Cu,-1.5572171373,0,-1.1123627598
 Cu,0,0,1.9740946813
 Cu,1.5572171373,0,-1.1123627598
 Br,0,0,4.5486217363

	<p>MP2= -1681.03783540 NIMAG= 0</p> <p>N,-0.6868875416,0,-10.7843400592</p> <p>N,0.6868875416,0,-10.7843400592</p> <p>N,-2.4986172386,0,-7.6378798611</p> <p>N,-1.8179093903,0,-6.4491386349</p> <p>N,1.8179093903,0,-6.4491386349</p> <p>N,2.4986172386,0,-7.6378798611</p> <p>C,-1.1068506079,0,-12.0892274237</p> <p>C,1.1068506079,0,-12.0892274237</p> <p>C,-3.835790008,0,-7.3628324554</p> <p>C,-2.7308856168,0,-5.4316056356</p> <p>C,2.7308856168,0,-5.4316056356</p> <p>C,3.835790008,0,-7.3628324554</p> <p>C,0,0,-12.9525787217</p> <p>C,-4.0277723418,0,-5.97036245</p> <p>C,4.0277723418,0,-5.97036245</p> <p>H,-2.1718351127,0,-12.3184215305</p> <p>H,2.1718351127,0,-12.3184215305</p> <p>H,-4.5588709084,0,-8.1770696907</p> <p>H,-2.3941291424,0,-4.3959897279</p> <p>H,2.3941291424,0,-4.3959897279</p> <p>H,4.5588709084,0,-8.1770696907</p> <p>H,0,0,-14.0503572796</p> <p>H,-4.9725520185,0,-5.4298067155</p> <p>H,4.9725520185,0,-5.4298067155</p> <p>Cu,-1.6026166437,0,-9.223906773</p> <p>Cu,0,0,-6.4404417938</p> <p>Cu,1.6026166437,0,-9.223906773</p> <p>Br,0,0,-16.5973768637</p>
	<p>MP2= -1464.65453414 NIMAG= 0</p> <p>X</p> <p>X,1,r21</p> <p>X,1,r21,2,120.</p> <p>X,1,r21,2,120.,3,180.,0</p> <p>N,2,r52,1,90.,3,0.,0</p> <p>N,2,r52,1,90.,4,0.,0</p> <p>N,3,r52,1,90.,2,0.,0</p> <p>N,3,r52,1,90.,4,0.,0</p> <p>N,4,r52,1,90.,3,0.,0</p> <p>N,4,r52,1,90.,2,0.,0</p> <p>C,5,r115,2,a1152,1,180.,0</p> <p>C,6,r115,2,a1152,1,180.,0</p>

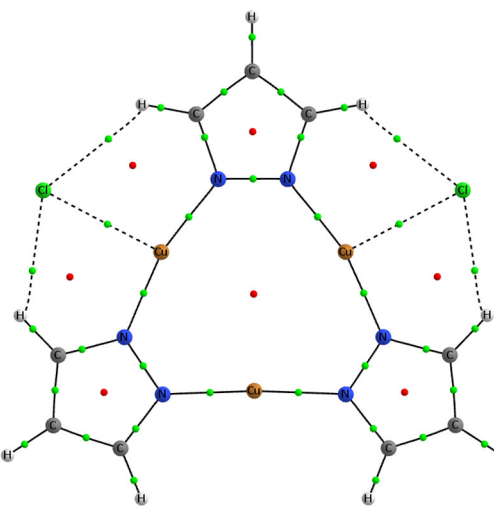
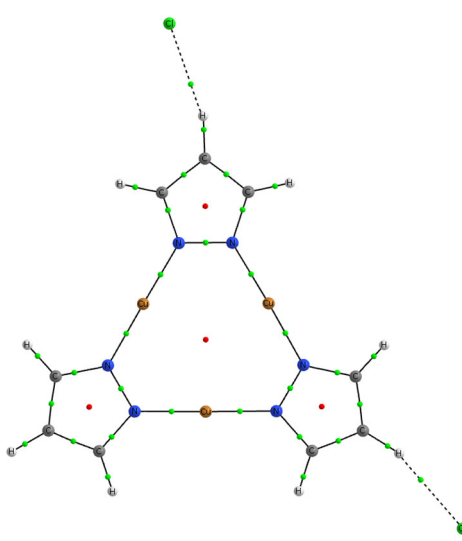
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	C,8,r115,3,a1152,1,180.,0
	C,9,r115,4,a1152,1,180.,0
	C,10,r115,4,a1152,1,180.,0
	C,1,r171,3,120.,2,0.,0
	C,1,r171,4,120.,3,0.,0
	C,1,r171,2,120.,4,0.,0
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	H,12,r2011,6,a20115,2,180.,0
	H,13,r2011,7,a20115,3,180.,0
	H,14,r2011,8,a20115,3,180.,0
	H,15,r2011,9,a20115,4,180.,0
	H,16,r2011,10,a20115,4,180.,0
	H,1,r261,3,120.,2,0.,0
	H,1,r261,4,120.,3,0.,0
	H,1,r261,2,120.,4,0.,0
	Cu,1,r291,3,60.,2,0.,0
	Cu,1,r291,4,60.,3,0.,0
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	F,1,rcl,2,90.,3,90.,0
	F,1,rcl,2,90.,3,-90.,0
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	r52=0.68717892
	r115=1.36470525
	r171=4.70335136
	r2011=1.08937051
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	r291=1.75190017
	a1152=108.11361618
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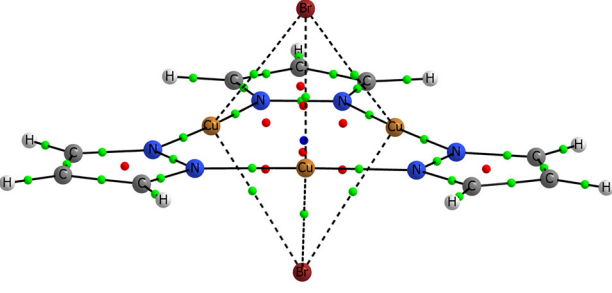
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	N,-0.6825049132,0.,2.500369
	N,2.5117690541,0.,-0.6574584142
	N,1.8252602157,0.,-1.8465266022
	N,-1.8372804008,0.,-1.8537194166
	N,-2.5066355295,0.,-0.6591179071
	C,1.1006344469,0.,3.8164786151
	C,-1.1327118858,0.,3.7944577166
	C,3.8504478917,0.,-0.9330566956
	C,2.7332747475,0.,-2.8680573423
	C,-2.7548502102,0.,-2.861416699
	C,-3.852452719,0.,-0.9162715902
	C,-0.0257314844,0.,4.6663883114
	C,4.037921737,0.,-2.3312952018
	C,-4.0540765637,0.,-2.3109100367
	H,2.1783254272,0.,3.9893293367
	H,-2.2035044489,0.,4.0008596095
	H,4.5434671965,0.,-0.0905160651
	H,2.3501228101,0.,-3.8894999809
	H,-2.365697836,0.,-3.8811498261
	H,-4.5665982832,0.,-0.0921389748
	H,-0.0421725102,0.,5.7570279473
	H,4.9831465557,0.,-2.8770210052
	H,-5.0068187077,0.,-2.8419915086
	Cu,1.8143024254,0.,1.0509451009
	Cu,-0.0029939426,0.,-2.096704541
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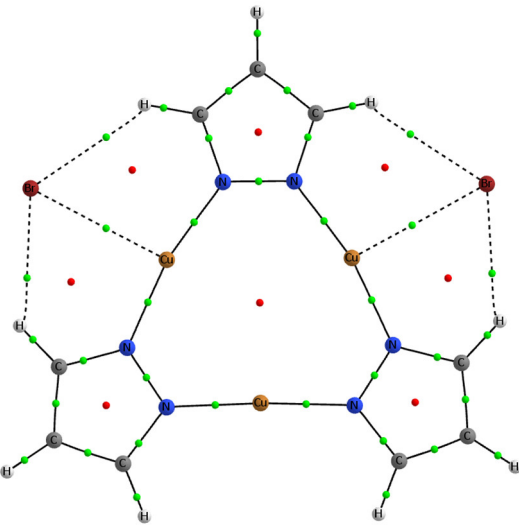
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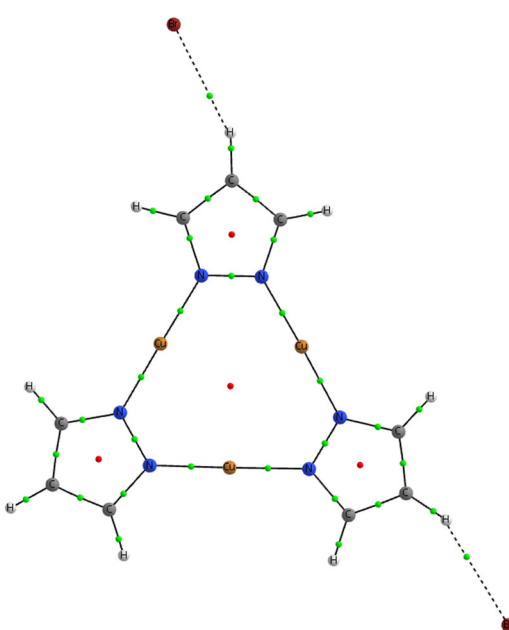
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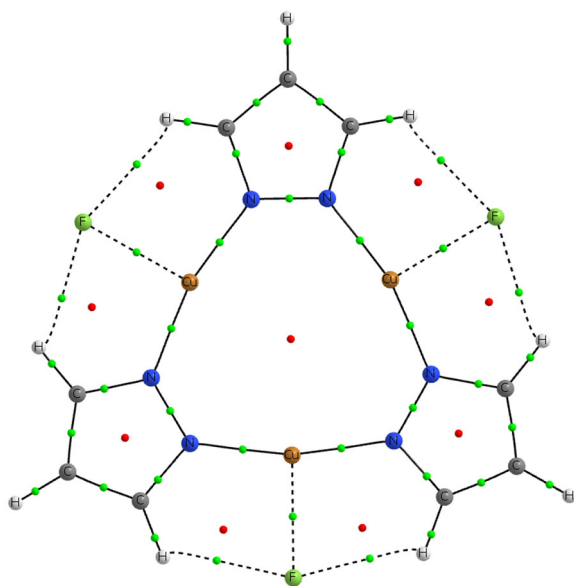
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	C,8,r115,3,a1152,1,180.,0
	C,9,r115,4,a1152,1,180.,0
	C,10,r115,4,a1152,1,180.,0
	C,1,r171,3,120.,2,0.,0
	C,1,r171,4,120.,3,0.,0
	C,1,r171,2,120.,4,0.,0
	H,11,r2011,5,a20115,2,180.,0
	H,12,r2011,6,a20115,2,180.,0
	H,13,r2011,7,a20115,3,180.,0
	H,14,r2011,8,a20115,3,180.,0
	H,15,r2011,9,a20115,4,180.,0
	H,16,r2011,10,a20115,4,180.,0
	H,1,r261,3,120.,2,0.,0
	H,1,r261,4,120.,3,0.,0
	H,1,r261,2,120.,4,0.,0
	Cu,1,r291,3,60.,2,0.,0
	Cu,1,r291,4,60.,3,0.,0
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	Cl,1,rcl,2,90.,3,90.,0
	Cl,1,rcl,2,90.,3,-90.,0
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	r52=0.68522631
	r115=1.36423941
	r171=4.71051379
	r2011=1.08973696
	r261=5.80182159
	r291=1.77597194
	a1152=108.19693856
	a20115=119.70143651
	rcl=2.04332573

	<p>MP2= -2184.75417433 NIMAG= 0 N,0.7106717196,0.,2.5552085806 N,-0.6575304768,0.,2.476269808 N,2.510318538,0.,-0.65385345 N,1.821412967,0.,-1.8470729005 N,-1.8575396829,0.,-1.8930640532 N,-2.4732777987,0.,-0.6686968074 C,1.0581217499,0.,3.8750016858 C,-1.169216918,0.,3.7461131759 C,3.8495251073,0.,-0.9344670254 C,2.7340347366,0.,-2.8665530227 C,-2.8267890246,0.,-2.8538611586 C,-3.8288376348,0.,-0.8604850344 C,-0.1065249215,0.,4.6680635264 C,4.0340888282,0.,-2.3290822709 C,-4.0959240611,0.,-2.2417784751 H,2.1187047465,0.,4.1262126374 H,-2.2486923008,0.,3.8988780029 H,4.554198113,0.,-0.1030664731 H,2.3663572405,0.,-3.8925180232 H,-2.5140525921,0.,-3.8979584523 H,-4.5008735472,0.,-0.0020143437 H,-0.1703945117,0.,5.7563332671 H,4.9785630358,0.,-2.8743747089 H,-5.0703280978,0.,-2.7306006578 Cu,1.8178413009,0.,1.0623716145 Cu,-0.011120156,0.,-2.1054825539 Cu,-1.5031726613,0.,0.8678571406 Cl,4.053175986,0.,2.4655466819</p>
	<p>MP2= -2184.74426696 NIMAG= 0 N,0.6845829697,0.,2.4234402938 N,-0.6845829697,0.,2.4234402938 N,2.499640814,0.,-0.7222221747 N,1.8187363245,0.,-1.9148471021 N,-1.8187363245,0.,-1.9148471021 N,-2.499640814,0.,-0.7222221747 C,1.1128299442,0.,3.7204594977 C,-1.1128299442,0.,3.7204594977 C,3.842013863,0.,-0.9994484106 C,2.7471323694,0.,-2.9234615078 C,-2.7471323694,0.,-2.9234615078 C,-3.842013863,0.,-0.9994484106 C,0.,0.,4.5795374915</p>

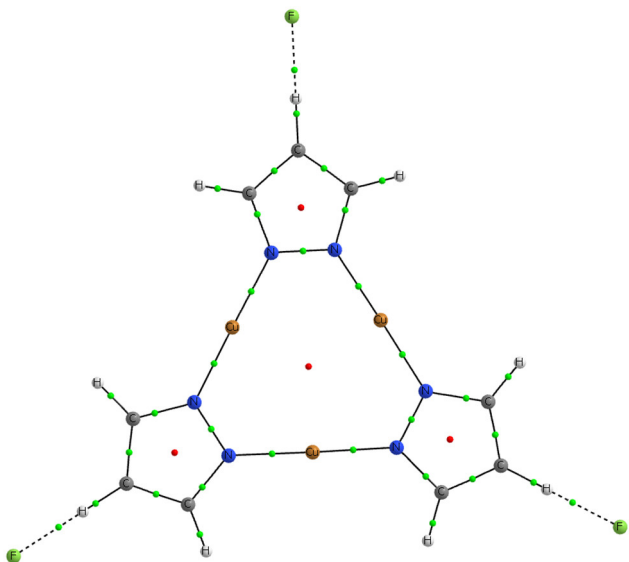
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	MP2= -2096.70196565 NIMAG= 0 X X,1,r21 X,1,r21,2,120. X,1,r21,2,120.,3,180.,0 N,2,r52,1,90.,3,0.,0 N,2,r52,1,90.,4,0.,0 N,3,r52,1,90.,2,0.,0 N,3,r52,1,90.,4,0.,0 N,4,r52,1,90.,3,0.,0 N,4,r52,1,90.,2,0.,0 C,5,r115,2,a1152,1,180.,0 C,6,r115,2,a1152,1,180.,0 C,7,r115,3,a1152,1,180.,0 C,8,r115,3,a1152,1,180.,0 C,9,r115,4,a1152,1,180.,0 C,10,r115,4,a1152,1,180.,0 C,1,r171,3,120.,2,0.,0 C,1,r171,4,120.,3,0.,0 C,1,r171,2,120.,4,0.,0 H,11,r2011,5,a20115,2,180.,0 H,12,r2011,6,a20115,2,180.,0 H,13,r2011,7,a20115,3,180.,0 H,14,r2011,8,a20115,3,180.,0 H,15,r2011,9,a20115,4,180.,0 H,16,r2011,10,a20115,4,180.,0

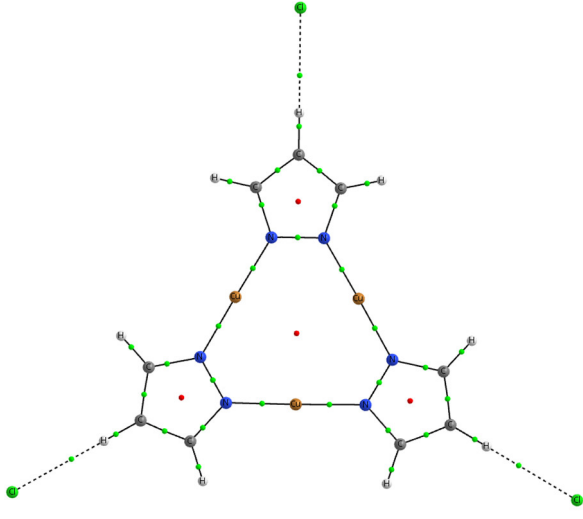
	H,1,r261,3,120.,2,0.,0 H,1,r261,4,120.,3,0.,0 H,1,r261,2,120.,4,0.,0 Cu,1,r291,3,60.,2,0.,0 Cu,1,r291,4,60.,3,0.,0 Cu,1,r291,2,60.,4,0.,0 Br,1,rcl,2,90.,3,90.,0 Br,1,rcl,2,90.,3,-90.,0 r21=2.5388156 r52=0.6843305 r115=1.36410625 r171=4.70280233 r2011=1.08968088 r261=5.79387384 r291=1.77861966 a1152=108.25139646 a20115=119.75793801 rcl=2.28093476
	MP2= -2096.73373352 NIMAG= 0 N,0.7393114761,0.,2.5344823242 N,-0.6294307014,0.,2.4591910189 N,2.5348832805,0.,-0.6684485026 N,1.8463350247,0.,-1.8610490652 N,-1.8252703401,0.,-1.9075036818 N,-2.4444372458,0.,-0.6844925322 C,1.0928980976,0.,3.8525930866 C,-1.135305385,0.,3.7309509228 C,3.8739311705,0.,-0.9477480452 C,2.7577394689,0.,-2.8810487835 C,-2.7899944346,0.,-2.8727740597 C,-3.7987509719,0.,-0.8822721571 C,-0.0693571591,0.,4.6482677876 C,4.0566076977,0.,-2.3420835462 C,-4.0601965672,0.,-2.2640688322 H,2.1536097496,0.,4.104014218 H,-2.2140332558,0.,3.887961268 H,4.5807292503,0.,-0.1181438731 H,2.3926802207,0.,-3.907955962 H,-2.4773756954,0.,-3.9170878621 H,-4.4740898549,0.,-0.0265715898 H,-0.128454298,0.,5.7364900757 H,5.0006614837,0.,-2.8871332537 H,-5.032173283,0.,-2.7570003527

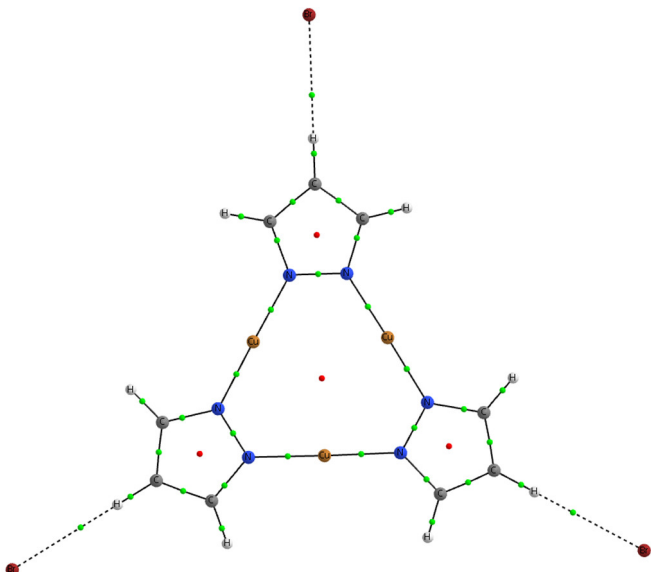
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Table S4. Electron density properties (au) at the intermolecular BCPs in the 1:1 complexes.

1:1 Cu complexes

Configuration	Atoms	Dist	Rho	Lap	H
Apical	Cu25-F28	2.1354	0.0522	0.2611	-0.0071
Planar	F28-Cu26	2.0158	0.0683	0.3678	-0.0121
Planar	H19-F28	2.2785	0.0148	0.0541	0.0004
CH(4)	H22-F28	1.5510	0.0608	0.1809	-0.0107
Apical	Cl28-Cu25	2.5561	0.0392	0.1336	-0.0034
Planar	Cl28-Cu26	2.4297	0.0507	0.1711	-0.0084
Planar	H19-Cl28	2.5748	0.0141	0.0429	0.0009
CH(4)	H22-Cl28	2.3572	0.0192	0.0495	0.0005
Apical	Br28-Cu25	2.6924	0.0362	0.1012	-0.0040
Planar	Br28-Cu26	2.5745	0.0455	0.1243	-0.0080
Planar	H19-Br28	2.6652	0.0140	0.0404	0.0008
CH(4)	Br28-H22	2.5470	0.0160	0.0379	0.0003

1: 1 Ag complexes

Configuration	Atoms	Dist	Rho	Lap	H
Apical	F28-Ag25	2.379	0.0422	0.1823	-0.0045
Planar	F28-Ag26	2.256	0.0545	0.2623	-0.0048
Planar	H19-F28	2.483	0.0094	0.0355	0.0009
CH(4)	H22-F28	1.554	0.0605	0.1800	-0.0105
Apical	Cl28-Ag25	2.758	0.0341	0.1118	-0.0026
Planar	Cl28-Ag26	2.623	0.0443	0.1474	-0.0051
Planar	H19-Cl28	2.790	0.0094	0.0272	0.0007
CH(4)	H22-Cl28	2.366	0.0188	0.0486	0.0005
Apical	Br28-Ag25	2.856	0.0337	0.0935	-0.0039
Planar	Br28-Ag26	2.722	0.0434	0.1177	-0.0072
Planar	H19-Br28	2.889	0.0093	0.0263	0.0008
CH(4)	H22-Br28	2.556	0.0157	0.0373	0.0003

1: 1 Au complexes

Configuration	Atoms	Dist	Rho	Lap	H
Apical	Au25-F28	2.558	0.0358	0.1296	-0.0036
Planar	F28-Au26	2.434	0.0454	0.1776	-0.0046
Planar	H19-F28	2.336	0.0126	0.0433	0.0004
CH(4)	H22-F28	1.508	0.0676	0.1866	-0.0155
Apical	Cl28-Au25	3.017	0.0253	0.0738	-0.0005
Planar	Cl28-Au26	2.956	0.0283	0.0817	-0.0008

Planar	H19-Cl28	2.614	0.0127	0.0351	0.0006
CH(4)	H22-Cl28	2.317	0.0208	0.0537	0.0005
Apical	Br28-Au25	3.127	0.0246	0.0637	-0.0010
Planar	Br28-Au26	3.088	0.0265	0.0666	-0.0014
Planar	H19-Br28	2.706	0.0127	0.0336	0.0006
CH(4)	H22-Br28	2.507	0.0173	0.0406	0.0003

Table S5. Barriers (kJ mol⁻¹) and interhalogen distance (Å) in the maximum of the dissociation curve (Figure S1) of the 1:2 apical complexes.

	Barrier			X...X distance		
	F⁻	Cl⁻	Br⁻	F⁻	Cl⁻	Br⁻
Au	33.0	7.5	8.7	4.9	6.2	6.7
Ag	88.6	56.4	59.0	5.4	6.3	6.8
Cu	95.6	29.6	23.7	4.7	5.7	6.2

Table S6. Interatomic X...X distances (Å) in the 1:2 complexes.

F⁻	1:2 apical	1:2 planar	1:2 CH(4)
Au	3.534	12.219*	13.360
Ag	3.165	8.343	13.602
Cu	2.697	7.370	13.156
Cl⁻			
Au	5.206	9.323	15.182
Ag	4.330	8.886	15.484
Cu	4.087	8.324	15.023
Br⁻			
Au	5.483	9.510	15.699
Ag	4.627	9.097	16.019
Cu	4.562	8.801	15.537

* In this complex, the F(-) anions are interacting with the C(3)-H.

Table S7. Anion-Anion repulsion corrected binding energies (kJ/mol) for the 1:2 complexes.

F⁻	1:2 apical	1:2 planar	1:2 CH(4)
Au	-280.1	-149.4	-143.6
Ag	-485.4	-245.5	-120.7
Cu	-549.9	-270.8	-125.9
Cl⁻			
Au	-127.4	-125.1	-75.7
Ag	-297.6	-182.2	-60.5
Cu	-246.5	-164.8	-64.4
Br⁻			
Au	-133.0	-125.9	-69.7
Ag	-285.0	-176.7	-55.5
Cu	-210.5	-147.3	-59.1

Table S8. Electron density properties (au) at the intermolecular BCPs in the 1:2 complexes.

1:2 Cu complexes

Configuration	Atoms	Dist	Rho	Lap	H
Apical	F28-F29	2.6975	0.0197	0.0744	-0.0010
Apical	Cu25-F28	2.2109	0.0442	0.2059	-0.0055
Planar	F28-Cu25	2.0895	0.0577	0.2947	-0.0087
Planar	F28-H18	2.4934	0.0095	0.0383	0.0011
Planar	H16-F28	2.2599	0.0153	0.0538	0.0002
CH(4)	F28-H23	1.6591	0.0471	0.1519	-0.0043
Apical	Cl28-Cu25	2.7073	0.0293	0.0928	-0.0012
Planar	Cl28-Cu25	2.6392	0.0333	0.1072	-0.0020
Planar	Cl28-H18	2.6170	0.0127	0.0376	0.0008
Planar	H16-Cl28	2.5495	0.0146	0.0430	0.0008
CH(4)	Cl28-H23	2.5325	0.0138	0.0352	0.0004
Apical	Br28-Cu25	2.8924	0.0252	0.0650	-0.0014
Planar	Cu25-Br28	2.9624	0.0222	0.0539	-0.0011
Planar	H18-Br28	2.7206	0.0123	0.0340	0.0007
Planar	H16-Br28	2.6397	0.0144	0.0392	0.0006
CH(4)	Br28-H23	2.7562	0.0110	0.0275	0.0005

1:2 Ag complexes

Configuration	Atoms	Dist	Rho	Lap	H
Apical	Ag26-F28	2.437	0.0372	0.1526	-0.0042
Planar	F28-Ag25	2.327	0.0467	0.2100	-0.0046
Planar	H16-F28	2.179	0.0173	0.0555	-0.0004
CH(4)	F28-H23	1.660	0.0470	0.1514	-0.0043
Apical	Cl28-Ag25	2.845	0.0287	0.0923	-0.0015
Planar	Cl28-Ag25	2.734	0.0354	0.1156	-0.0028
Planar	H16-Cl28	2.720	0.0106	0.0301	0.0006
Planar	Cl28-H18	2.971	0.0068	0.0200	0.0007
CH(4)	Cl28-H23	2.538	0.0137	0.0348	0.0004
Apical	Br28-Ag25	2.949	0.0282	0.0785	-0.0023
Planar	Br28-Ag25	2.849	0.0340	0.0932	-0.0039
Planar	Br28-H18	3.001	0.0075	0.0216	0.0008
Planar	H16-Br28	2.827	0.0103	0.0286	0.0007
CH(4)	Br28-H23	2.775	0.0107	0.0269	0.0005

1:2 Au complexes

Configuration	Atoms	Dist	Rho	Lap	H
Apical	Au25-F28	2.613	0.0320	0.1118	-0.0032

Planar	F28-H16	1.592	0.0552	0.1725	-0.0074
CH(4)	F28-H23	1.619	0.0517	0.1635	-0.0061
Apical	Cl28-Au25	3.226	0.0174	0.0482	0.0002
Planar	Au26-Cl29	3.325	0.0148	0.0391	0.0003
Planar	H16-Cl28	2.591	0.0130	0.0340	0.0005
Planar	Cl28-H18	2.977	0.0065	0.0179	0.0005
CH(4)	Cl28-H23	2.478	0.0153	0.0391	0.0005
Apical	Br28-Au25	3.339	0.0169	0.0436	0.0001
Planar	Br29-Au26	3.455	0.0140	0.0349	0.0003
Planar	H16-Br28	2.727	0.0120	0.0304	0.0005
Planar	H18-Br28	2.996	0.0074	0.0198	0.0006
CH(4)	Br28-H23	2.696	0.0123	0.0304	0.0005

Table S9. Interatomic distances (Å) of the anions in the 1:3 complexes.

F(-)	Planar	CH(4)
Au		13.361
Ag	8.158	13.573
Cu	7.450	13.141
Cl(-)	planar	CH(4)
Au		14.866
Ag	9.038	15.169
Cu		14.733
Br(-)	planar	CH(4)
Au		15.226
Ag	9.353	15.559
Cu		15.120

Table S10. Anion-Anion repulsion corrected binding energies (kJ/mol) in the 1:3 complexes.

F(-)	Planar	CH(4)
Au		-175.8
Ag	-286.3	-146.8
Cu	-307.4	-153.3
Cl(-)	planar	CH(4)
Au		-92.3
Ag	-201.0	-71.7
Cu		-76.6
Br(-)	planar	CH(4)
Au		-85.6
Ag	-193.4	-66.0
Cu		-70.7

Table S11. Electron density properties at the intermolecular BCPs in the 1:3 complexes.

1:3 Cu complexes

Configuration	Atoms	Dist	Rho	Lap	H
Planar	F28-Cu25	2.2108	0.0443	0.2049	-0.0053
Planar	F28-H16	2.3875	0.0116	0.0425	0.0007
CH(4)	F30-H22	1.7813	0.0357	0.1149	-0.0018
CH(4)	H22-Cl30	2.7431	0.0093	0.0231	0.0003
CH(4)	Br30-H22	2.9699	0.0074	0.0182	0.0005

1:3 Ag complexes

Configuration	Atoms	Dist	Rho	Lap	H
Planar	Ag27-F30	2.411	0.0392	0.1624	-0.0042
Planar	F28-H16	2.461	0.0098	0.0350	0.0007
CH(4)	F30-H22	1.777	0.0360	0.1160	-0.0019
Planar	Cl30-Ag27	3.025	0.0204	0.0615	-0.0002
Planar	H16-Cl28	2.863	0.0081	0.0225	0.0006
CH(4)	Cl28-H23	2.740	0.0094	0.0232	0.0003
Planar	Br30-Ag27	3.238	0.0166	0.0448	0.0001
Planar	H16-Br28	2.942	0.0082	0.0223	0.0007
CH(4)	H24-Br29	2.969	0.0074	0.0182	0.0005

1:3 Au complexes

Configuration	Atoms	Dist	Rho	Lap	H
CH(4)	F30-H22	1.735	0.0395	0.1280	-0.0025
CH(4)	H22-Cl30	2.651	0.0110	0.0273	0.0003
CH(4)	H22-Br30	2.864	0.0089	0.0217	0.0005

Table S12. Anion-Metal distances in the CSD search.**Cu-F**

Refcode	Distances (Å)		
HUXWUU	2.383	2.579	2.482
HUXWUU	2.605	2.536	2.448
	Average	Maximum	Minimum
	2.506	2.605	2.383

Cu-Cl

Refcode	Distances (Å)		
JALKIT	2.622	2.424	2.486
OBOQAY	2.359	2.545	2.923
OBOQEC	2.361	2.549	2.931
OBOQIG	2.354	2.560	2.977
RETQIR	2.500	2.584	2.558
RETQIR	2.628	2.501	2.614
RUYGUN	2.461	2.453	3.056
RUYGUN	2.641	2.965	2.350
RUYGUN	2.486	2.398	3.039
RUYGUN	2.756	2.756	2.341
RUYHAU	2.600	2.986	2.357
UWOMAW	2.626	2.502	2.630
UWOMAW	2.648	2.761	2.581
VADYAB	2.623	2.603	2.603
VAZCUX	2.527	2.631	2.666
VAZCUX	2.604	2.527	2.564
	Average	Maximum	Minimum
	2.609	3.056	2.341

Cu-Br

Refcode	Distances (Å)		
ELODIS	2.722	3.063	2.504
ELODOY	2.652	2.750	2.645
ELODOY	2.698	2.638	2.806
	Average	Maximum	Minimum
	2.720	3.063	2.504

Figure S1. Energy profiles (kJ/mol) as a function of the X-X distance (Å) in the 1:2 apical complexes. Only one of the X anions in move further away from the (Pz-M)₃X⁻ system.

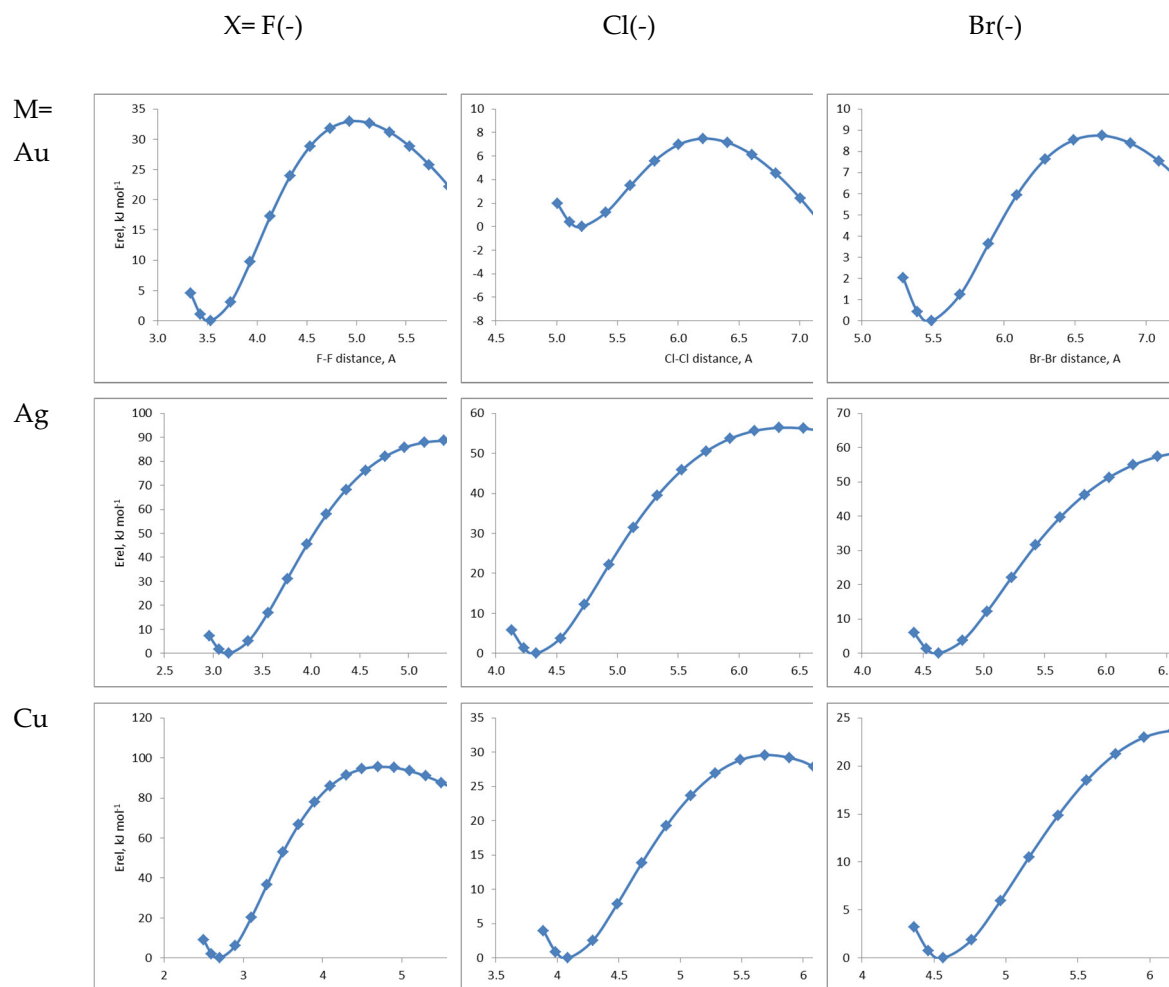
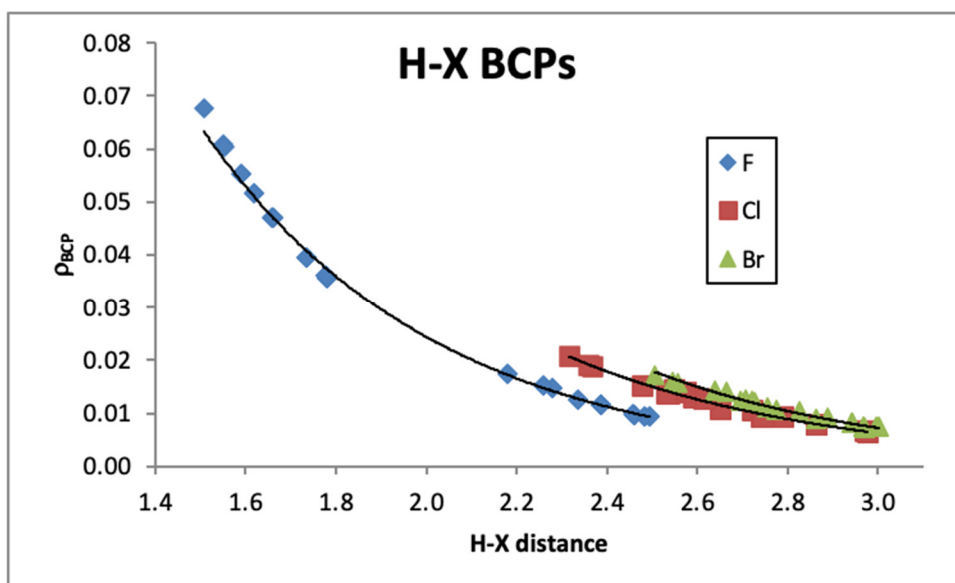
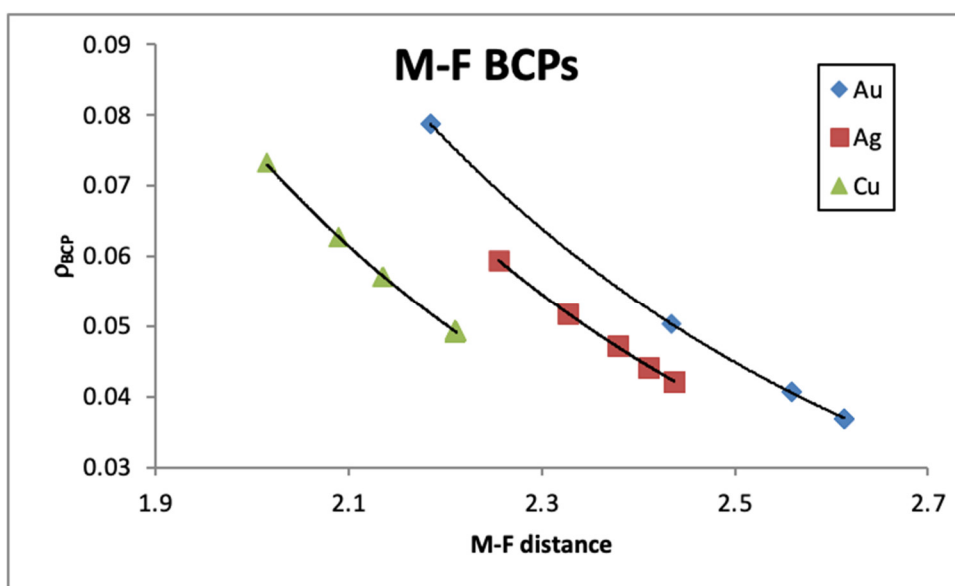


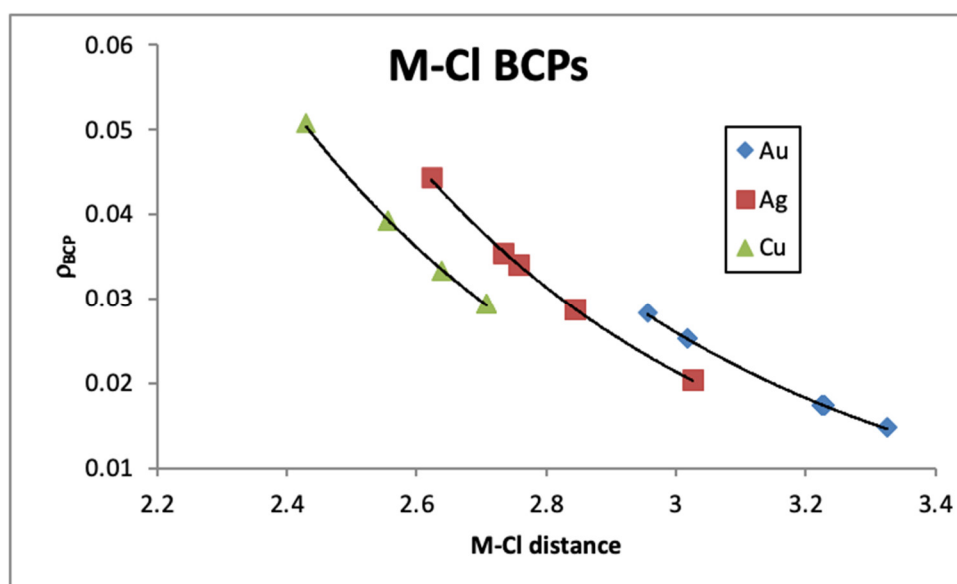
Figure S2. Electron density at the BCP (au) vs. the interatomic distance (Å).



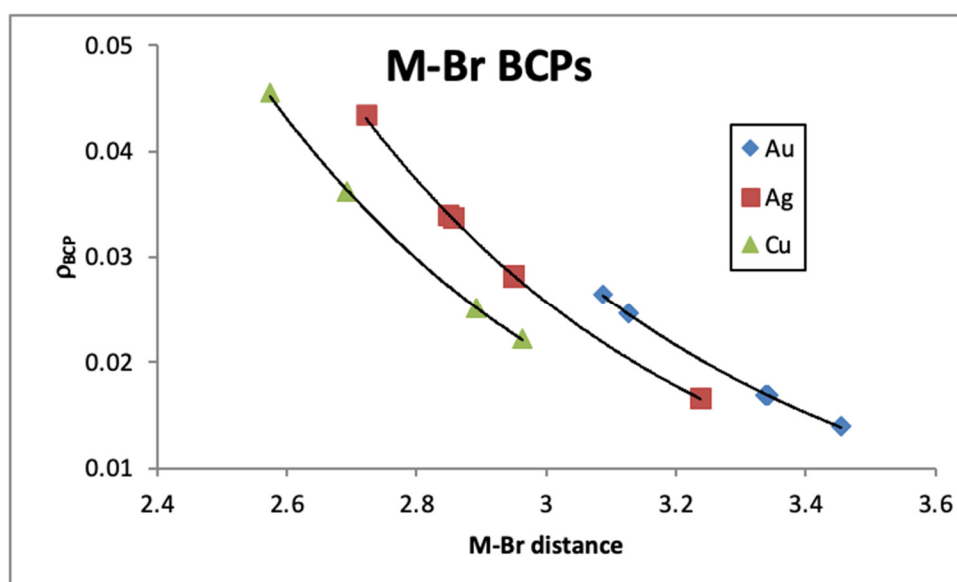
The exponential relationships show R^2 values of 0.998 (H-F), 0.98 (H-Cl) and 0.98 (H-Br).



The exponential relationships show R^2 values > 0.999 .



The exponential relationships show R^2 values > 0.999 .



The exponential relationships show R^2 values > 0.99 .