Supporting Information for

Theoretical Investigation on the Nature of π(B≡B)···M Interaction in Coinage Metal π-Diborene Complexes

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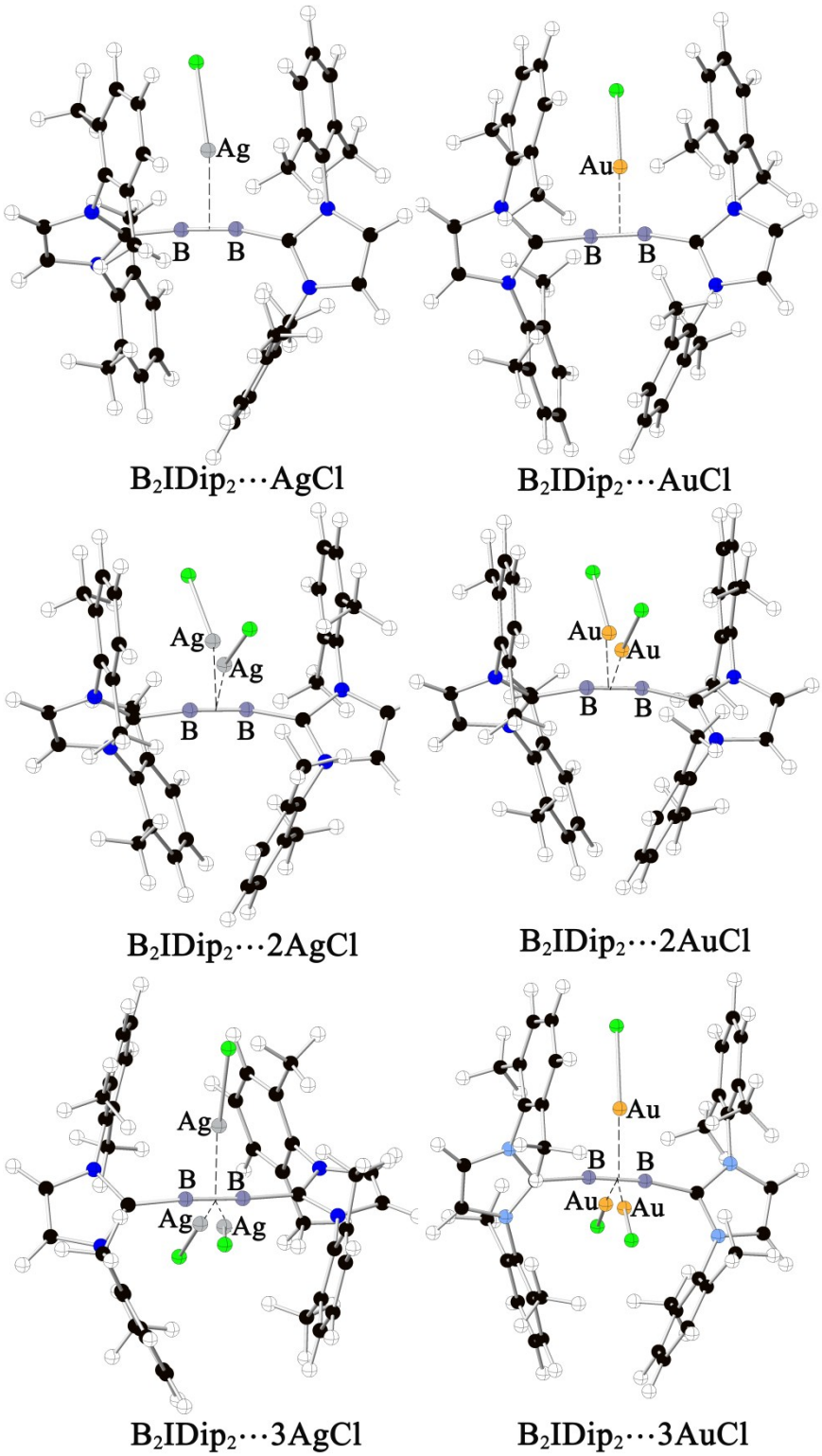
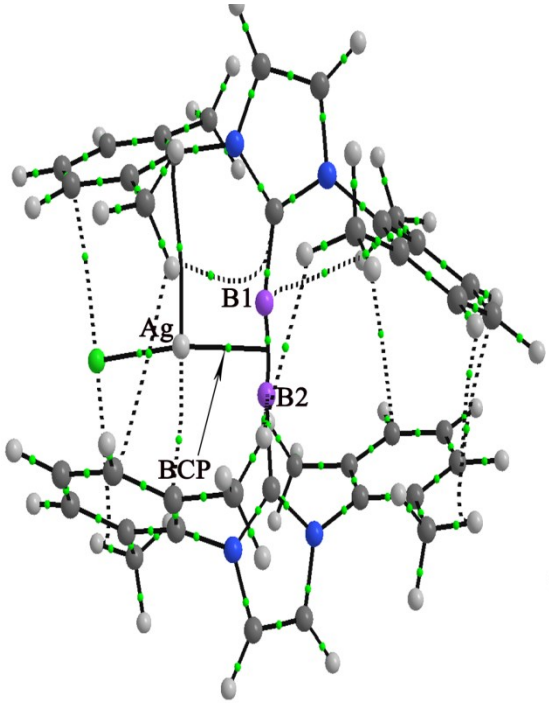
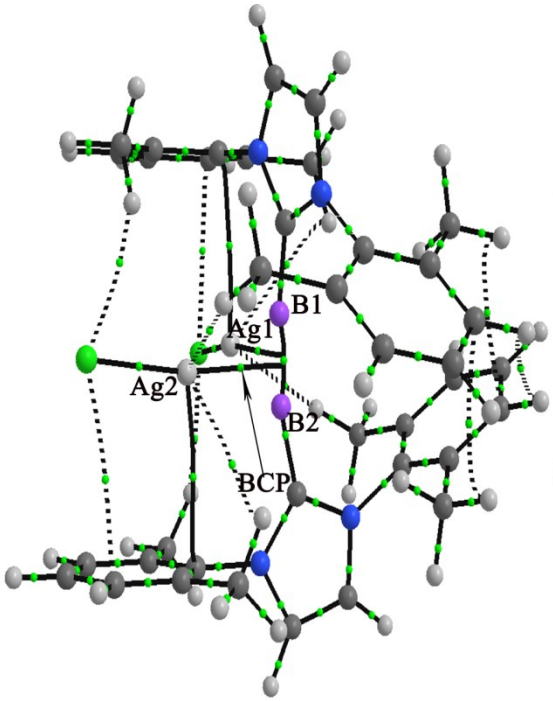


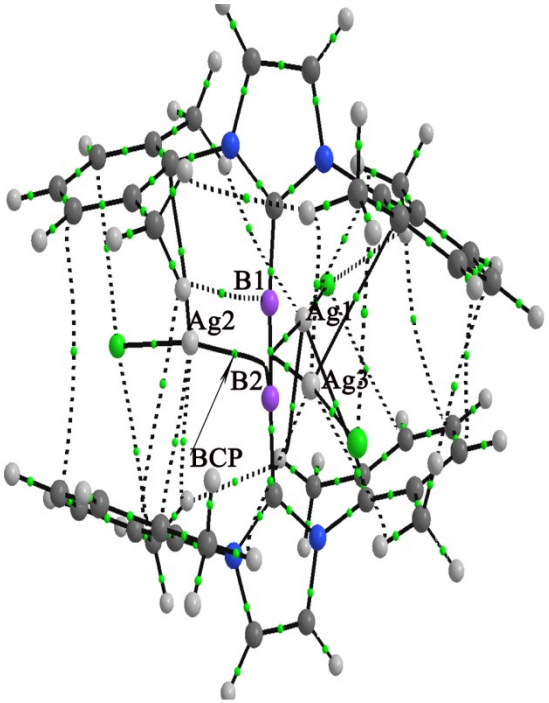
Fig. S1 Geometries of $B_2IDip_2\cdots nMCl$(n=1, 2, 3; M=Ag and Au)



$B_2IDip_2\cdots AgCl$



$B_2IDip_2\cdots 2AgCl$



$B_2IDip_2\cdots 3AgCl$

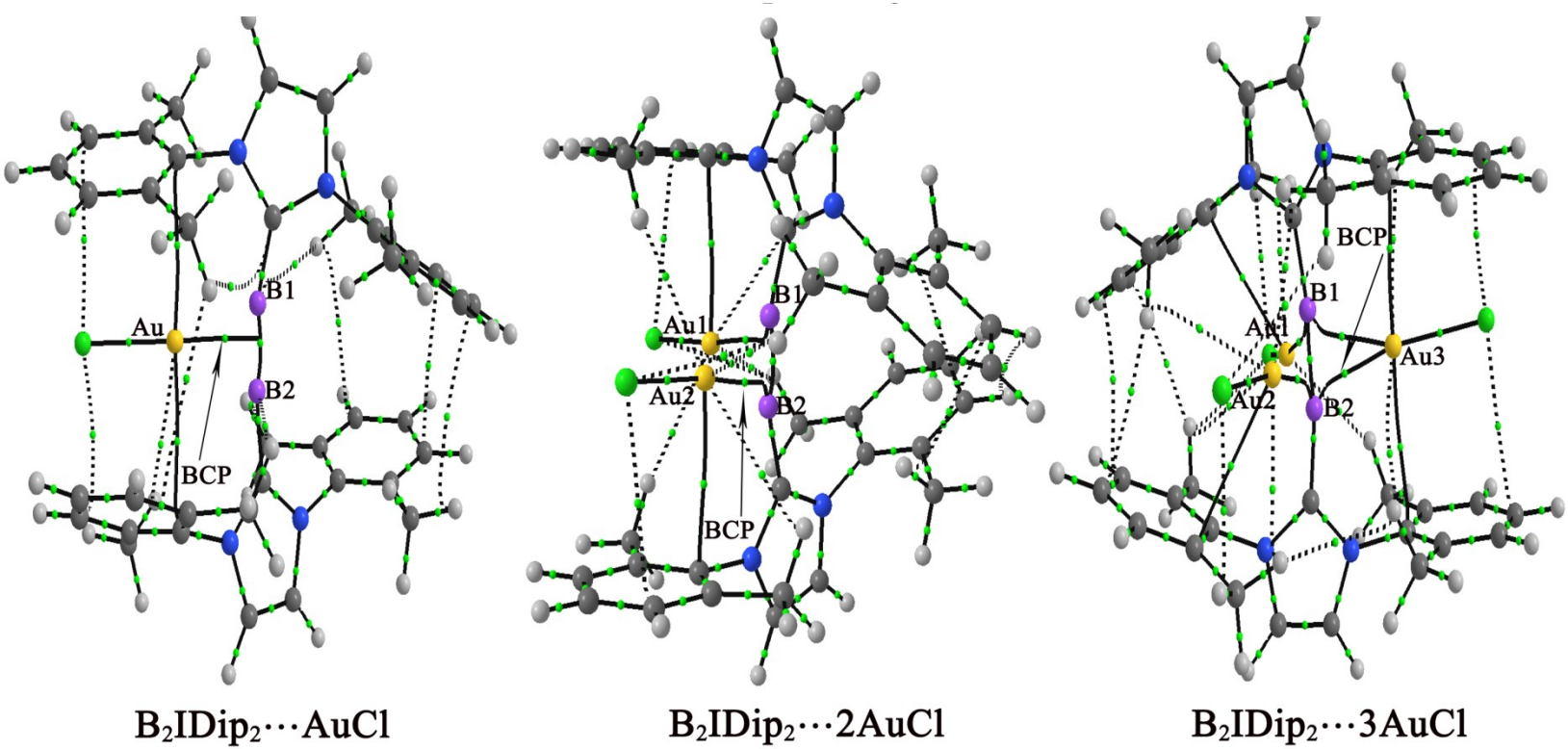
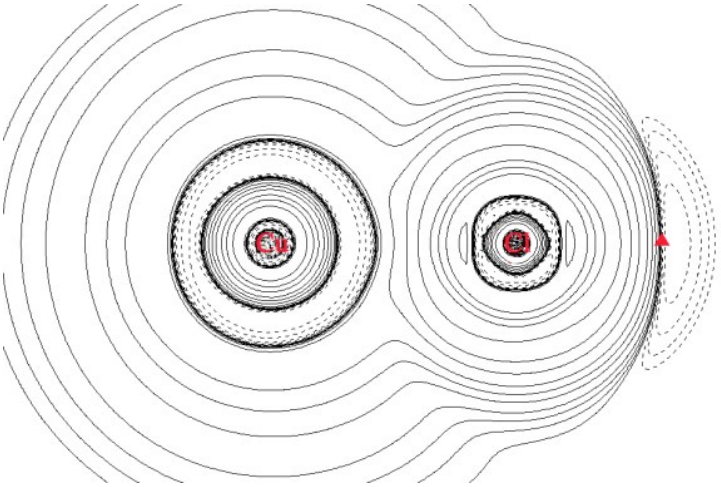
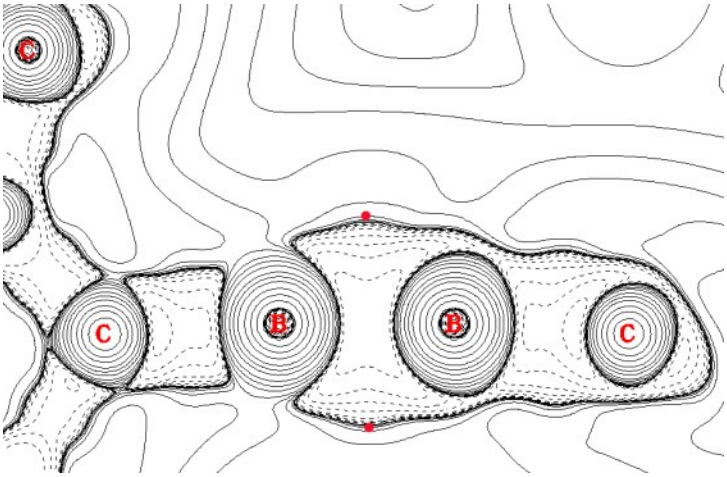


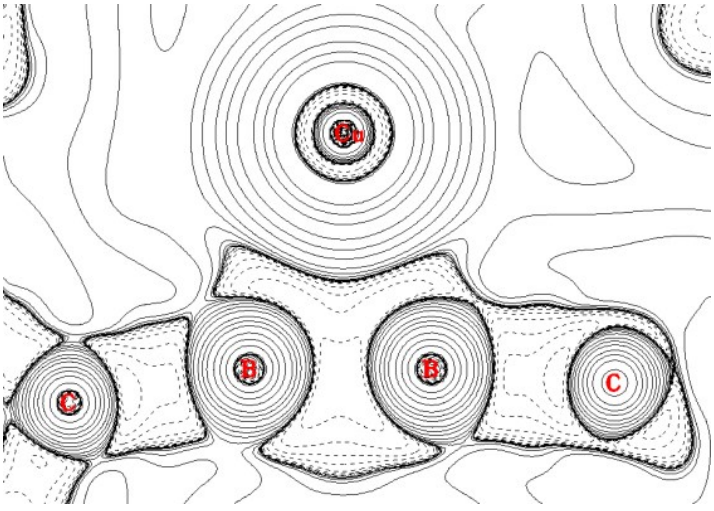
Fig. S2 Molecular graphs of $B_2IDip_2\cdots nMCl$(n=1, 2, 3; M=Ag and Au)



(a)

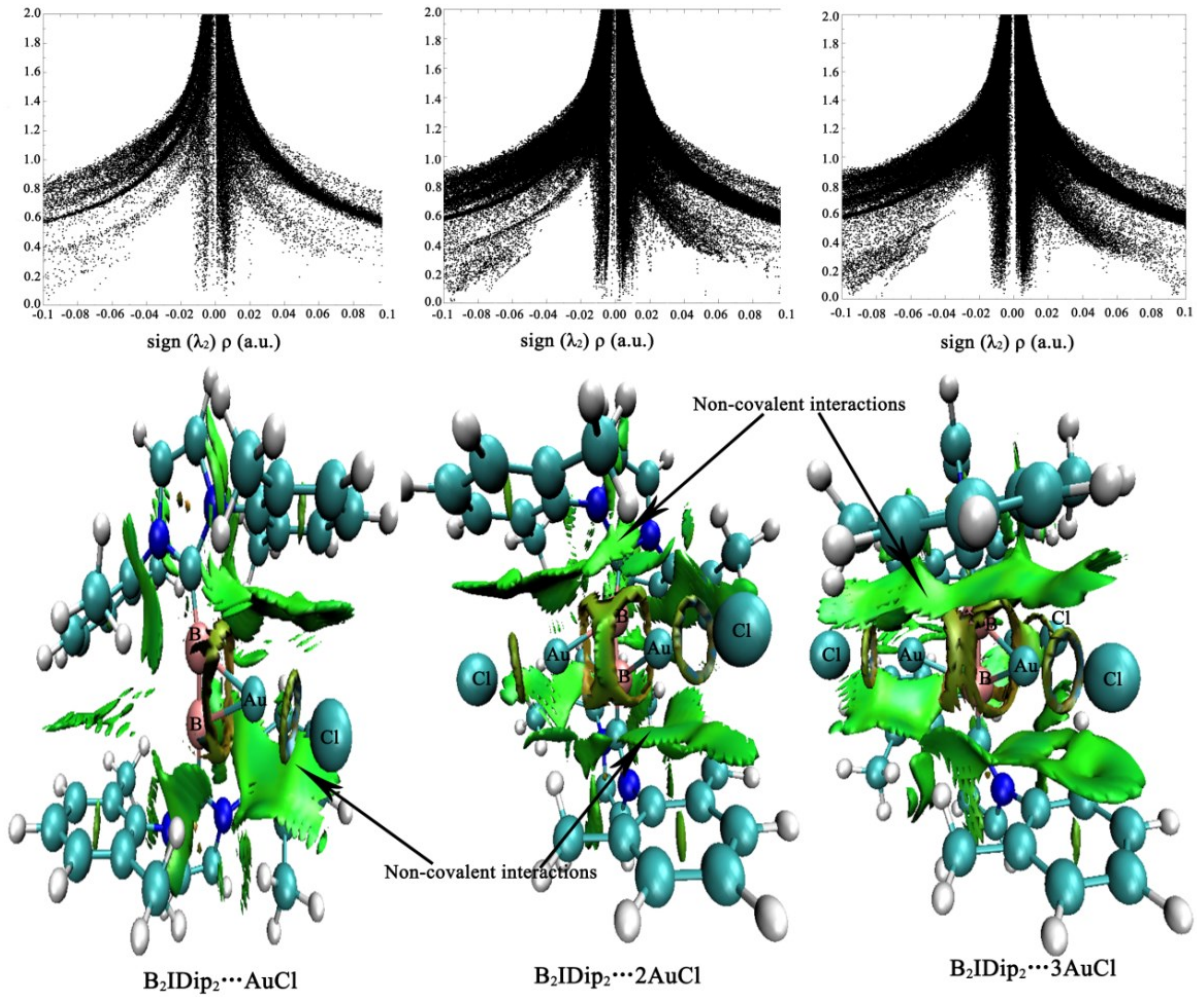


(b)



(c)

Fig. S3 Contour maps of Laplacian for CuCl(a), B_2IDip_2 (b) and B_2IDip_2 ···CuCl(c) (▲:charge depletion region; ●: charge concentration region)


sign (λ2) ρ (a.u.)
sign (λ2) ρ (a.u.)
sign (λ2) ρ (a.u.)
Non-covalent interactions
Non-covalent interactions
B2IDip2···AuCl
B2IDip2···2AuCl
B2IDip2···3AuCl

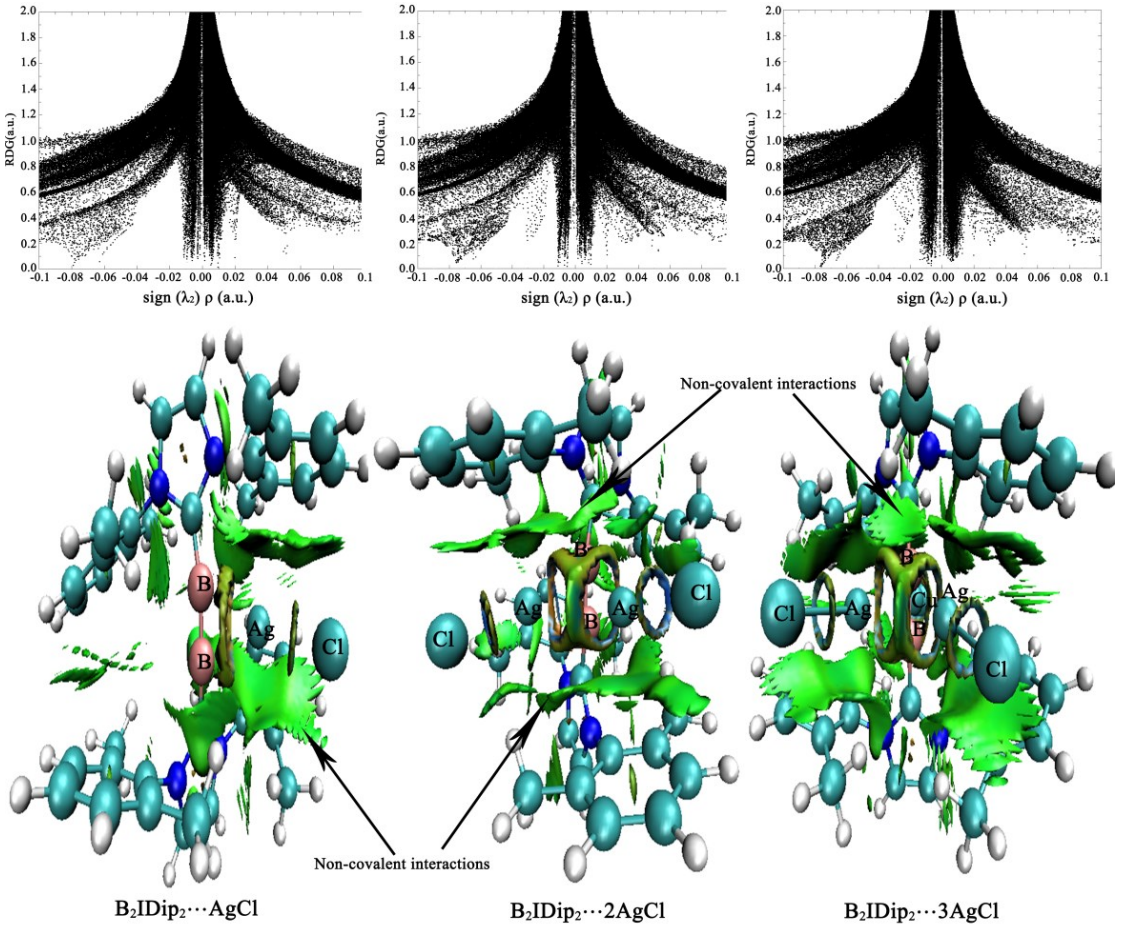


Fig. S4 Plots of the reduced density gradient versus the electron density multiplied by the sign of the second Hessian eigenvalue (above) and isosurfaces generated for s=0.05 a.u. (below) for $B_2IDip_2\cdots nMCl$(n=1, 2, 3; M=Ag and Au)

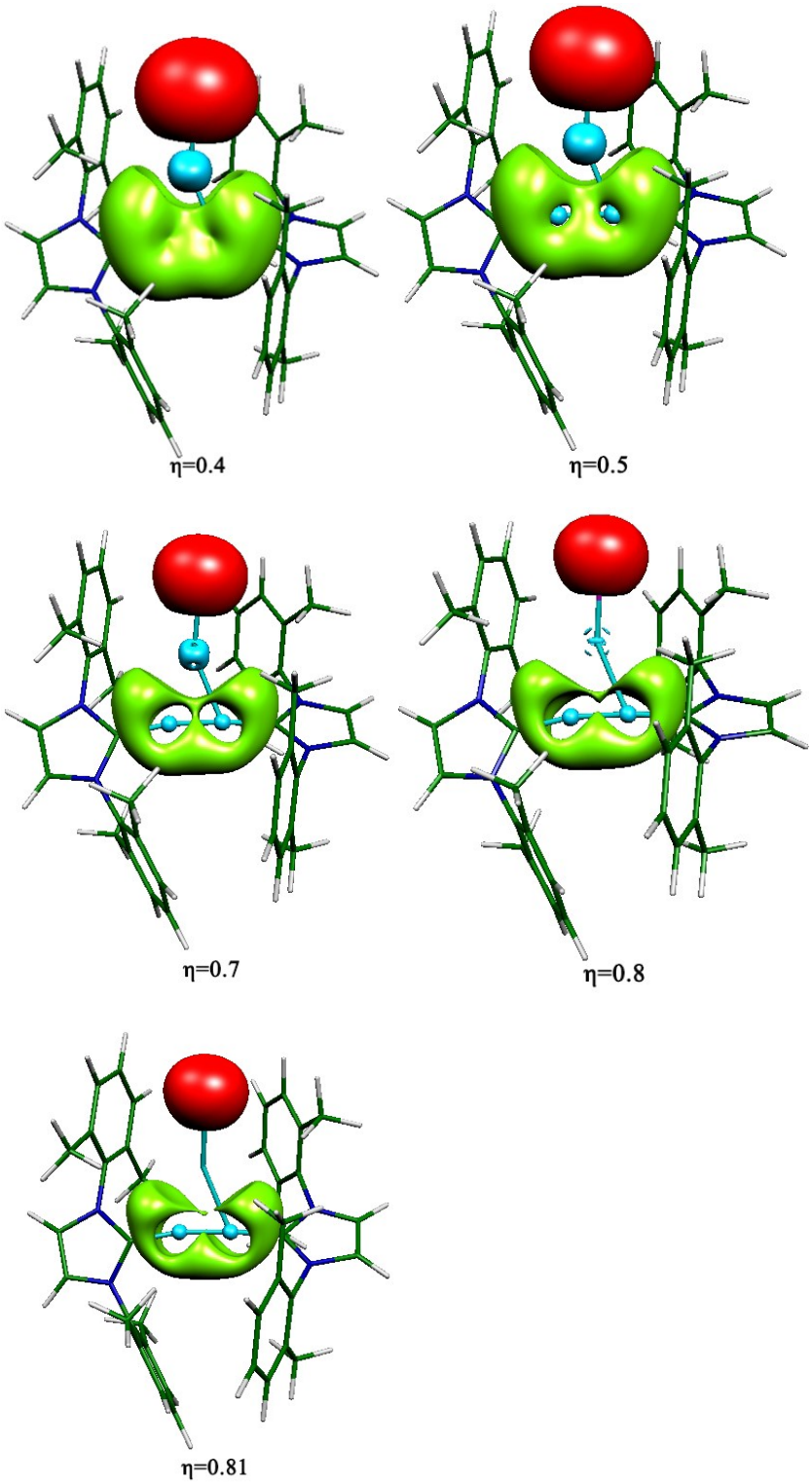


Fig. S5 ELF localization domains of B_2IDip_2···CuCl at different isosurfaces

Table S1 Geometry parameters of the studied complexes optimized at M06L/def2-SVP level (in Å)

□	CuCl	AgCl	AuCl	2CuCl	2AgCl	2AuCl	3CuCl	3AgCl	3AuCl
R_{B-B}	1.480	1.483	1.494	1.504(1.486)	1.506	1.529	1.544(1.526)	1.547	1.618
$^{a}\Delta R_{B-B}$	0.011	0.014	0.025	0.035	0.037	0.060	0.075	0.078	0.149
R_{B-C}	1.493	1.495	1.500	1.516(1.546)	1.522	1.531	1.538(1.561)	1.539	1.562
$^{a}\Delta R_{B-C}$	0.016	0.018	0.023	0.039	0.045	0.054	0.061	0.062	0.085
	2.190	2.414	2.423	2.189(2.161)	2.403	2.405	2.173(2.123)	2.394	2.395
R_{M-Cl}				2.190(2.158)	2.403	2.405	2.172(2.123)	2.399	2.394
							2.190(2.192)	2.389	2.402
R_{B1-M1}	2.066	2.246	2.189	2.061(2.087)	2.281	2.188	2.094(2.056)	2.299	2.195
FSR_{B1-M1}	0.926	0.940	0.916	0.924	0.954	0.915	0.939	0.962	0.918
R_{B2-M2}	2.066	2.258	2.188	2.061(2.079)	2.259	2.211	2.065(2.107)	2.247	2.201
FSR_{B2-M1}	0.927	0.945	0.916	0.924	0.945	0.925	0.926	0.940	0.921
R_{B1-M3}				2.082(2.075)	2.260	2.211	2.113(2.086)	2.283	2.209
FSR_{B1-M2}				0.934	0.946	0.925	0.948	0.955	0.924
R_{B2-M1}				2.081(2.078)	2.280	2.188	2.117(2.086)	2.255	2.203
FSR_{B2-M2}				0.933	0.954	0.916	0.949	0.944	0.922
R_{B1-M2}							2.105(2.107)	2.266	2.185
FSR_{B1-M3}							0.944	0.948	0.914
R_{B2-M3}							2.064(2.056)	2.278	2.186
FSR_{B2-M3}	□	□	□	□	□	□	0.925	0.953	0.915

The numbers in parentheses are experimental geometry parameters from Ref. 23

Table S2 Geometry parameters of the studied complexes optimized at M06L/def2-TZVP level (in Å)

	π-CuCl	π-AgCl	π-AuCl	π-2CuCl	π-2AgCl	π-2AuCl	π-3CuCl	π-3AgCl	π-3AuCl
R_{B-B}	1.466	1.467	1.480	1.491	1.493	1.516	1.534	1.538	1.612
[a]ΔR_{B-B}	-0.003	-0.002	0.011	0.022	0.024	0.047	0.065	0.069	0.143
R_{B-C}	1.491	1.500	1.505	1.513	1.516	1.525	1.535	1.535	1.558
[a]ΔR_{B-C}	0.011	0.020	0.025	0.033	0.036	0.045	0.055	0.055	0.078
R_{M-Cl}	2.169	2.398	2.393	2.164	2.387	2.377	2.146	2.374	2.360
				2.164	2.385	2.377	2.158	2.368	2.363
							2.159	2.378	2.367
R_{B1-M1}	2.054	2.241	2.189	2.074	2.298	2.192	2.115	2.294	2.190
FSR_{B1-M1}	0.921	0.938	0.916	0.930	0.962	0.917	0.948	0.960	0.916
R_{B1-M2}	2.054	2.259	2.183	2.074	2.263	2.211	2.049	2.250	2.199
FSR_{B1-M2}	0.921	0.945	0.913	0.930	0.947	0.925	0.919	0.942	0.920
R_{B1-M2}				2.088	2.281	2.211	2.114	2.280	2.206
FSR_{B1-M2}				0.936	0.954	0.925	0.948	0.954	0.923
R_{B2-M1}				2.088	2.279	2.192	2.136	2.251	2.197
FSR_{B2-M1}				0.936	0.953	0.917	0.958	0.942	0.919
R_{B2-M2}							2.114	2.265	2.183
FSR_{B2-M2}							0.948	0.948	0.913
R_{B2-M3}							2.054	2.270	2.181
FSR_{B2-M3}							0.921	0.950	0.913

[a]ΔR is the difference between the R in B_2IDip_2 and that in complex

Table S3 The optimized xyz coordinations for B_2IDip_2, MCl(M=Cu, Ag, and Au), and nine studied complexes at M06L/def2-SVP level

B_2IDip_2			
B	-0.65959400	0.35905000	-0.23439900
B	0.59846600	-0.38642600	-0.37320400
N	-1.99858100	2.12202700	1.03521800
C	-1.89094800	1.10407100	0.09892100
N	-3.17280700	0.97481700	-0.41225300
C	-3.29149800	2.61925800	1.06487000
H	-3.57873400	3.42097600	1.73875000
C	-0.17998900	3.68155000	1.47703600
C	-0.91242400	2.54503300	1.85633500
N	3.08952500	-0.84583300	-0.91788200
C	-4.01964100	1.91191500	0.16490700
H	-5.07160700	1.96640700	-0.09800700
N	2.10765100	-2.29810100	0.39117900
C	0.87507200	4.08405600	2.30239200
H	1.45905400	4.96654200	2.02595100
C	1.19773000	3.36271900	3.44900700
H	2.02607600	3.68961400	4.08256000
C	0.47667800	2.21998000	3.78513400
H	0.74214600	1.64708700	4.67815500
C	-0.59120900	1.78455100	2.99325500
C	-3.54492100	-0.01205400	-1.36835000
C	-3.95105100	-2.30476200	-1.94753800
H	-3.99541000	-3.36064400	-1.66571700
C	-3.59233300	-1.36302800	-0.97637300
C	-4.25287200	-1.91772200	-3.24962600
H	-4.53128200	-2.67063100	-3.99100200
C	-4.19489200	-0.57458600	-3.61259800
H	-4.41549400	-0.27367100	-4.64035100
C	-3.83279300	0.40246200	-2.68090400
C	1.87181800	-1.13329800	-0.32256800
C	1.13658700	-2.87834300	1.26046300
C	-0.73031200	-4.33930000	1.61751000
H	-1.46360000	-5.05403600	1.23322000
C	0.20764700	-3.79053500	0.73631200
C	3.32715200	0.31696300	-1.70568500
C	3.46412400	0.16562900	-3.09637600
C	3.69474000	1.31277900	-3.86111400
C	3.76682700	2.56639500	-3.25864600
H	3.94007600	3.45492500	-3.87062700
C	3.61366800	2.69200300	-1.88135000
H	3.66823400	3.67831100	-1.41170600
C	3.39489900	1.57141400	-1.07183700
C	3.42378700	-2.70443200	0.23685700
C	4.03114700	-1.80897300	-0.58219300
C	-0.75021400	-3.97197700	2.96049700

H	-1.49139700	-4.41026200	3.63336100
C	0.16108600	-3.03793000	3.44746300
H	0.12659700	-2.73143500	4.49676300
C	1.11772200	-2.46648300	2.60278800
C	-1.34137600	0.53192000	3.30587300
H	-2.43097600	0.68640700	3.29972900
H	-1.13023500	-0.23625100	2.53955100
H	-1.05887900	0.12447300	4.28517900
C	-3.25582800	-1.78491200	0.41476700
H	-2.16134500	-1.77163600	0.56797400
H	-3.67441000	-1.10240200	1.16936400
H	-3.61970300	-2.79910400	0.62522300
C	-3.71538400	1.84332400	-3.06402600
H	-2.75365200	2.26602900	-2.73604900
H	-3.79339000	1.97458400	-4.15021900
H	-4.49735800	2.46618600	-2.60189800
C	3.32346300	-1.18286200	-3.72783300
H	4.14348000	-1.86420300	-3.45223600
H	2.39353300	-1.67589500	-3.40575200
H	3.30991100	-1.11226300	-4.82228800
C	3.22312300	1.70824600	0.40421300
H	3.75110100	0.91600000	0.95600500
H	3.58730800	2.67994600	0.76227000
H	2.15659800	1.61865100	0.68049900
C	0.19184300	-4.09920600	-0.72461000
H	-0.10883600	-3.20296800	-1.29449700
H	1.18417400	-4.38790500	-1.10166900
H	-0.51309300	-4.90626300	-0.96044600
C	2.05229500	-1.39887700	3.07124400
H	3.10740600	-1.65094500	2.88382600
H	1.85650400	-0.45887400	2.52663700
H	1.93766100	-1.20271000	4.14495400
C	-0.48942400	4.38389300	0.19440100
H	-0.33844800	3.70412800	-0.66022200
H	-1.53518000	4.72261600	0.13981100
H	0.15567200	5.25918600	0.04903000
H	5.05231400	-1.75857700	-0.94778800
H	3.80683600	-3.59551700	0.72552100
H	3.79767600	1.21734600	-4.9453850
CuCl			
Cl	0.00000000	0.00000000	-1.31303200
Cu	0.00000000	0.00000000	0.76970800
AgCl			
Cl	0.00000000	0.00000000	-1.70470500
Ag	0.00000000	0.00000000	0.61659500
AuCl			
Cl	0.00000000	0.00000000	-1.87914400
Au	0.00000000	0.00000000	0.40437300

B_2IDip_2…CuCl

B	0.33516100	-0.66954900	0.12551000
B	0.05999400	0.77603300	-0.03308900
N	-0.12098100	-2.99832000	1.13633700
C	0.65487400	-2.10286500	0.44260300
N	1.77961000	-2.80293000	0.09820300
C	0.51148700	-4.22357100	1.21121800
H	0.06021300	-5.06773700	1.72347800
Cl	-3.05816900	-1.08921800	-2.13678900
C	-2.50387700	-3.13792200	0.70593500
C	-1.46295800	-2.69663800	1.53799200
N	-1.07471900	3.07548800	-0.29127500
C	1.70053200	-4.10409500	0.56148700
H	2.49603100	-4.82228100	0.38773500
N	1.03701800	3.14473000	0.24178700
C	-3.80318000	-2.74266000	1.03658500
H	-4.62441600	-3.03164700	0.37710100
C	-4.04331100	-1.95588100	2.15839100
H	-5.06522600	-1.65139600	2.39772600
C	-2.98967800	-1.54074300	2.96957400
H	-3.18377000	-0.91448300	3.84502000
C	-1.67010200	-1.89194600	2.66861400
C	2.80972400	-2.27140600	-0.74115800
C	4.98139800	-1.29519000	-0.98727700
H	5.90517500	-0.91125700	-0.54550900
C	3.97771100	-1.77861800	-0.14182100
C	4.80499500	-1.28194800	-2.36811100
H	5.59919800	-0.89944100	-3.01445400
C	3.61857900	-1.74513000	-2.93122600
H	3.47896500	-1.71874200	-4.01500200
C	2.59083500	-2.25224800	-2.12870900
C	0.01171500	2.26836500	-0.04291500
C	2.36026700	2.74772100	0.60475800
C	4.53894200	1.96067200	-0.00066500
H	5.24539900	1.62189200	-0.76271600
C	3.23747400	2.29438400	-0.39326900
C	-2.39944500	2.57991600	-0.52024400
C	-2.87622500	2.49135100	-1.83581400
C	-4.18473000	2.03683300	-2.01737400
C	-4.96547500	1.65815900	-0.93223600
C	-4.45561000	1.72444100	0.36079700
H	-5.06699000	1.40788900	1.21012500
C	-3.16123800	2.19357800	0.59666600
C	0.58544200	4.45130600	0.18326000
C	-0.73100500	4.40671900	-0.15316500
C	4.93541000	2.05273700	1.33001500
H	5.95777000	1.78790000	1.61296400
C	4.03230200	2.47049600	2.30467300
H	4.33694800	2.51912400	3.35355100
C	2.72398300	2.82346900	1.95978900
C	-0.52079300	-1.38364600	3.47580500

H	0.22190100	-2.16716200	3.68785300	H	-1.77563600	1.50222500	2.07683200
H	0.01192000	-0.58898300	2.92316200	C	2.78159100	2.12815300	-1.80370800
H	-0.85703200	-0.96337200	4.43224200	H	2.11369200	1.25093400	-1.87351800
C	4.10347800	-1.71649700	1.34606100	H	2.19853000	2.99089200	-2.15948900
H	3.35630100	-1.02332600	1.76698200	H	3.62618100	1.97099600	-2.48602500
H	3.93417300	-2.69160000	1.82687600	C	1.72167200	3.22848200	2.99326100
H	5.09425300	-1.35693300	1.65008500	H	1.39133300	4.27223200	2.87543900
C	1.29881200	-2.72473100	-2.71212400	H	0.81332000	2.60933700	2.92689300
H	0.46829400	-2.04424800	-2.45026200	H	2.12864900	3.12568800	4.00654100
H	1.34821200	-2.77701100	-3.80610100	C	-2.21340500	-3.94211000	-0.51862900
H	1.01221700	-3.71976500	-2.33892500	H	-3.11856100	-4.09166900	-1.11658900
C	-1.97776800	2.76708900	-2.99712100	H	-1.49650900	-3.41432800	-1.16676500
H	-1.39347500	3.69175500	-2.88207800	H	-1.78513200	-4.92835900	-0.27804900
H	-1.25280800	1.94312000	-3.11075400	H	-5.97561000	1.27802800	-1.09899300
H	-2.54249000	2.83206400	-3.93490700	H	-4.57175100	1.93090000	-3.03314000
C	-2.58237200	2.24909500	1.97260800	H	-1.45380500	5.20051300	-0.31542100
H	-2.13528800	3.22953500	2.20019300	H	1.24753200	5.29198100	0.36771200
H	-3.34174200	2.03653000	2.73560200	Cu	-1.46136800	-0.38375900	-0.81360800

B_2IDip_2…2CuCl

B	0.20441500	0.74840500	0.07548100	C	0.30783900	4.44037300	0.60094300
B	0.20178600	-0.74854400	-0.07100400	H	-0.12532900	5.42105400	0.43078800
N	-0.25284500	3.30108100	0.06067500	Cl	-2.44698400	0.14826900	3.09060700
C	0.47043400	2.20146200	0.41714700	C	-2.67917200	3.38907900	-0.06770400
Cl	-2.44253200	-0.13646100	-3.08939500	C	-1.44729300	3.27584900	-0.73605000
N	1.49632000	2.67977200	1.18142000	N	-0.28035900	-3.29600300	-0.07834900

C	1.40545200	4.05246300	1.30436400
H	2.12965500	4.62222600	1.87853800
N	1.47497000	-2.68372600	-1.19314100
C	-3.83273500	3.39906600	-0.85693500
H	-4.80651400	3.47105300	-0.36613900
C	-3.75193300	3.30502600	-2.24371100
H	-4.66531700	3.30107300	-2.84219700
C	-2.51841100	3.18580800	-2.87159200
H	-2.46455100	3.06906600	-3.95562200
C	-1.33313300	3.16390900	-2.13102700
C	2.51657900	1.86436300	1.76912800
C	4.69068800	0.87605600	1.63420100
H	5.61975900	0.69101600	1.08752400
C	3.68500800	1.63508000	1.02784400
C	4.51353500	0.35225000	2.91276300
H	5.30860600	-0.24148600	3.37096100
C	3.32865700	0.57249900	3.60877700
H	3.19208300	0.15054600	4.60792600
C	2.29938200	1.34254200	3.05319000
C	0.45454200	-2.20104200	-0.42456700
C	2.50870900	-1.87696500	-1.76776700
C	4.69493300	-0.92048200	-1.60961100
H	5.62162200	-0.74986400	-1.05427800
C	3.67250200	-1.66555100	-1.01411500
C	-1.46706400	-3.26578300	0.72816900
C	-1.34275500	-3.14716600	2.12147300
C	-2.52365400	-3.16915200	2.87036900
C	-3.76118200	-3.29277600	2.25232800
C	-3.85211300	-3.38947900	0.86594500
H	-4.82944800	-3.46239300	0.38239000
C	-2.70454900	-3.37999100	0.06897800
C	1.36891100	-4.05413700	-1.32913300
C	0.26698700	-4.43633900	-0.62950000
C	4.53709800	-0.39230500	-2.88917600
H	5.34535600	0.18987200	-3.33908000
C	3.35498200	-0.59182400	-3.59597500
H	3.23343200	-0.16446300	-4.59474800
C	2.30911900	-1.34732900	-3.05132700
C	-0.01597500	2.94245300	-2.80166400
H	0.81089800	3.47877100	-2.31434600
H	0.23940100	1.86675800	-2.78166000
H	-0.04990200	3.24344600	-3.85607100
C	3.81094100	2.15476100	-0.36748600
H	3.09023500	1.64997200	-1.03417600
H	3.60342500	3.23369800	-0.43411200
H	4.81495900	1.98086600	-0.77340100
C	1.01541800	1.58615200	3.77367400
H	0.16031700	1.10096600	3.26930900
H	1.04699400	1.19565000	4.79764700
H	0.76541400	2.65652900	3.82912600
C	-0.02599800	-2.91592600	2.79063000
H	0.82673000	-3.31676500	2.22486400

H	0.14313100	-1.82982800	2.90735500	H	0.17630200	-1.06749800	-3.27924900
H	-0.00821800	-3.35085600	3.79840000	H	1.07060400	-1.17287600	-4.80313300
C	-2.77312600	-3.45094300	-1.42159800	C	-2.73752500	3.45961500	1.42317900
H	-2.28885800	-4.35546600	-1.82230900	H	-3.77414100	3.47226200	1.77933100
H	-3.81210900	-3.44930800	-1.77103300	H	-2.25437300	2.58412000	1.88925200
H	-2.28015800	-2.58310600	-1.89159600	H	-2.23749800	4.35666400	1.82123900
C	3.77393000	-2.19165100	0.38109800	H	-0.17644600	-5.41374000	-0.46746500
H	3.03882900	-1.69298100	1.03747100	H	2.08685200	-4.62638100	-1.90865200
H	3.56716100	-3.27152400	0.43732900	H	-2.46241400	-3.04843300	3.95363600
H	4.77008500	-2.01896900	0.80632600	H	-4.67015600	-3.28871200	2.85749000
C	1.02572600	-1.56594500	-3.78065400	Cu	-1.23922500	0.09922200	-1.27641000
H	0.75639800	-2.63129100	-3.84104600	Cu		-1.24205700	-0.09479900	1.27774000

B_2IDip_2…3CuCl

B	-0.15881800	0.83326400	0.04047200	C	-1.65421200	4.26238100	-0.12450000
B	-0.05295100	-0.70629000	0.10399800	H	-2.50241200	4.89644500	-0.36295000
N	0.25766100	3.35889600	0.47841100	N	-1.05882500	-2.87672700	1.13133200
C	-0.52986000	2.32205100	0.07803600	C	3.93787100	3.11787400	0.35043300
Cl	1.92635200	-0.25196900	3.58469000	H	4.73872800	3.14300500	-0.39115400
N	-1.71126900	2.89356500	-0.28840500	C	4.22212200	2.85175300	1.68721600
C	-0.41584900	4.55305200	0.35754300	H	5.25626800	2.68118600	1.99467300
H	0.04914900	5.49612400	0.62764300	C	3.20395700	2.78044700	2.63385000
Cl	3.46368500	0.50805300	-1.96005800	H	3.43085300	2.54011400	3.67430200
C	2.62125600	3.31327400	-0.07451500	C	1.86944000	2.96752600	2.26092300
C	1.62040100	3.21540300	0.90313200	C	-2.85374000	2.20114500	-0.81004500
N	0.78115100	-3.16250000	0.02523500	C	-4.89319400	1.01810900	-0.44500900

H	-5.62770300	0.57937600	0.23417300
C	-3.74902300	1.61141500	0.09567700
C	-5.10279700	0.98939800	-1.82214200
H	-5.99818500	0.50906600	-2.22423600
C	-4.17873800	1.55919100	-2.69176200
H	-4.32434300	1.49880600	-3.77209600
C	-3.03594500	2.19624200	-2.20047700
C	-0.11684700	-2.21310900	0.40650900
C	-2.27411200	-2.33306900	1.67106000
C	-4.58296500	-1.78845200	1.38696500
H	-5.46401600	-1.69815500	0.74735400
C	-3.37060200	-2.17908100	0.80620800
C	1.91555600	-2.96197600	-0.83901300
C	1.70240200	-3.05668200	-2.22428100
C	2.82479300	-2.93549800	-3.04722700
C	4.09233600	-2.75802900	-2.50212200
H	4.95449200	-2.65153800	-3.16366700
C	4.27014500	-2.69981400	-1.12444500
H	5.26710000	-2.54700900	-0.70546800
C	3.18152200	-2.79691300	-0.25517900
C	-0.74347000	-4.21766700	1.21056500
C	0.41060000	-4.39506500	0.51418900
C	-4.67992200	-1.54370300	2.75312400
H	-5.63868800	-1.24356100	3.18399400
C	-3.56588300	-1.68346300	3.57643300
H	-3.64490900	-1.48765000	4.64870900
C	-2.33572500	-2.09864300	3.05440000
C	0.74749300	2.90617700	3.24974400
H	0.22767500	3.87412900	3.33819400
H	-0.01216700	2.15916700	2.96201000
H	1.10963000	2.61193500	4.24097800
C	-3.46290400	1.59276300	1.56166200
H	-2.67827300	0.85042200	1.79573800
H	-3.09762800	2.56169300	1.93404400
H	-4.35265900	1.31997500	2.14199600
C	-2.01955200	2.81509900	-3.10450900
H	-1.01756700	2.39387200	-2.91956900
H	-2.24969200	2.61682700	-4.15699000
H	-1.94551300	3.90536500	-2.96407300
C	0.34095800	-3.32494800	-2.77537700
H	0.00530600	-4.34907100	-2.54193600
H	-0.41878200	-2.63668400	-2.37440500
H	0.31427500	-3.20063100	-3.86351100
C	3.34156800	-2.72280400	1.22578300
H	2.78948500	-1.87290100	1.66036000
H	2.96076900	-3.62236500	1.73457800
H	4.39321300	-2.60032400	1.50910000
C	-3.25371200	-2.41794200	-0.66255400
H	-2.74392800	-1.58106900	-1.17575800
H	-2.67411900	-3.32247400	-0.90060900
H	-4.23925700	-2.51613400	-1.13367900
C	-1.13737400	-2.29611500	3.92213100

H	-0.80707500	-3.34644800	3.93225900
H	-0.27058200	-1.70348100	3.58619100
H	-1.34525200	-2.00991500	4.95963300
C	2.27514400	3.59950100	-1.49962700
H	3.15688400	3.51937100	-2.14396100
H	1.54236200	2.87665300	-1.89224500
H	1.84071000	4.60547200	-1.62087800

B_2IDip_2…AgCl compound

B	0.46252900	-0.62451000	-0.02723200
B	0.08485600	0.80834500	-0.08283000
N	0.25563800	-2.98793500	0.99390200
C	0.90649300	-2.03722600	0.24557400
N	2.06339300	-2.64649200	-0.16416800
C	0.99091900	-4.15394400	1.03655900
H	0.64207800	-5.02776400	1.57826600
Cl	-3.63591200	-1.38261100	-1.79327700
C	-2.14838100	-3.30351400	0.86163900
C	-1.04597200	-2.78573500	1.55871500
N	-1.12263900	3.10389100	-0.08056000
C	2.12409200	-3.94339900	0.31434500
H	2.96257000	-4.59538400	0.08966700
N	0.98501600	3.14778700	0.46607000
C	-3.42094000	-3.00957100	1.36182700
H	-4.29587500	-3.35422700	0.80718300
C	-3.57144900	-2.23697000	2.50843100
Cl	-1.60625700	-0.49238500	-3.69340900
H	2.69170900	-2.97670600	-4.13067700
H	1.00278500	-5.28281600	0.31480700
H	-1.37612000	-4.91670500	1.74873200
Cu	-0.70791800	-0.09196400	-1.75569200
Cu	1.63726500	0.15129900	-0.83981300
Cu	1.06459200	0.15160600	1.61179700
H	-4.57398200	-2.00416200	2.87586900
C	-2.45622900	-1.74445700	3.18287600
H	-2.58268000	-1.13314400	4.08098800
C	-1.16379700	-2.00253200	2.71749700
C	3.04715300	-2.01623600	-0.98916100
C	5.18401500	-0.95399500	-1.19831200
H	6.10859000	-0.58346900	-0.74676100
C	4.22074200	-1.54893500	-0.37810700
C	4.96464700	-0.81179200	-2.56587700
H	5.72584500	-0.34091100	-3.19310800
C	3.77789700	-1.26080200	-3.13882100
H	3.60739800	-1.14028500	-4.21180200
C	2.78991800	-1.87751900	-2.36272400
C	-0.02185600	2.29179100	0.07144300
C	2.31333800	2.73449800	0.78907600
C	4.53224500	2.14498500	0.11001900
H	5.26804000	1.97862100	-0.68072600

C	3.22870400	2.50511700	-0.24956600
C	-2.43617200	2.63140300	-0.40009600
C	-2.85141600	2.65286300	-1.74078500
C	-4.13956700	2.19384300	-2.02396700
C	-4.96567100	1.72082100	-1.00982500
C	-4.52186600	1.69368700	0.30819500
H	-5.16198600	1.28561300	1.09471800
C	-3.24288500	2.14620600	0.64322200
C	0.50965900	4.44278800	0.56652300
C	-0.80387400	4.41483700	0.21893800
C	4.89409200	1.99985200	1.44573900
H	5.91898700	1.72021300	1.70434300
C	3.95582000	2.20359500	2.45513300
H	4.23772200	2.07335300	3.50352200
C	2.64417400	2.57505300	2.14486000
C	0.04302000	-1.42936300	3.38699900
H	0.83205000	-2.18148700	3.54069100
H	0.48619300	-0.63258700	2.76375300
H	-0.20776200	-0.99640400	4.36398300
C	4.39351500	-1.64157600	1.10385100
H	3.58114600	-1.10896400	1.62526800
H	4.37026600	-2.68016400	1.46785700
H	5.34407900	-1.19844700	1.42494300
C	1.50415200	-2.34520400	-2.96128000
H	0.67177900	-1.67547300	-2.68249600
H	1.55648700	-2.36984800	-4.05620800
H	1.22141600	-3.34882400	-2.61073100
C	-1.90822600	3.08629800	-2.81667100
H	-1.52550200	4.10629600	-2.65798200
H	-1.02734900	2.42398600	-2.85214200
H	-2.38575900	3.05524100	-3.80323900
C	-2.71096800	2.04437400	2.03601300
H	-2.21685200	2.96987600	2.37014900
H	-3.50596000	1.80217900	2.75266500
H	-1.95402900	1.24081200	2.09202100
C	2.81301900	2.60401000	-1.67968100
H	2.22240600	1.71581300	-1.96222900
H	2.17105300	3.47694000	-1.86887400
H	3.68017400	2.65843600	-2.34977400
C	1.61166000	2.78328400	3.20670700
H	1.30060000	3.83704200	3.28345800
H	0.69796500	2.20721200	2.99452500
H	1.98410000	2.47925400	4.19268500
C	-1.95906400	-4.07964700	-0.40112600
H	-2.91211300	-4.22565800	-0.92033100
H	-1.30028600	-3.53886400	-1.09954100
H	-1.50137100	-5.06547100	-0.21766500
Ag	-1.64465900	-0.46087100	-0.78737100
H	-5.95533400	1.33182900	-1.25633100
H	-4.47887900	2.17018100	-3.06214300
H	-1.54266700	5.20749700	0.15092100
H	1.15450700	5.26520700	0.86125500

B_2IDip_2…2AgCl

B	0.36088100	0.74323200	0.12191000
B	0.36092500	-0.74323200	-0.12177900
N	-0.09578200	3.30235700	0.28868500
C	0.60229100	2.16993200	0.59166300
Cl	-2.59715600	0.00665900	-3.39472500
N	1.58661200	2.57654700	1.44702500
C	0.43814900	4.38796100	0.95210400
H	0.01499200	5.38167600	0.84390500
Cl	-2.59819900	-0.00693800	3.39397200
C	-2.51691500	3.35569500	0.04889500
C	-1.25207400	3.34788600	-0.56188700
N	-0.09512200	-3.30243100	-0.28888200
C	1.49422200	3.93437000	1.67838300
H	2.18913200	4.44833000	2.33535100
N	1.58722900	-2.57609200	-1.44696000
C	-3.62896800	3.38262500	-0.79952100
H	-4.62845700	3.36840700	-0.35806800
C	-3.47481100	3.40871800	-2.18154000
H	-4.35482600	3.40228900	-2.82719900
C	-2.20636400	3.41384600	-2.75311700
H	-2.09616500	3.40363000	-3.83936400
C	-1.06141700	3.37957700	-1.95331000
C	2.59700100	1.71589600	1.98572400
C	4.75444700	0.70593100	1.77190000
H	5.67929000	0.54503400	1.21038500
C	3.76330300	1.52811100	1.22862200
C	4.56910000	0.09260700	3.00954500
H	5.35276100	-0.54972700	3.41912200
C	3.39441000	0.29130200	3.72870200
H	3.25686900	-0.19224100	4.69932300
C	2.37663900	1.11726500	3.23486600
C	0.60273200	-2.16981300	-0.59163600
C	2.59753900	-1.71525500	-1.98551800
C	4.75492400	-0.70517100	-1.77131900
H	5.67967800	-0.54424400	-1.20966600
C	3.76373000	-1.52741900	-1.22824500
C	-1.25141800	-3.34819800	0.56167000
C	-1.06076400	-3.37992100	1.95309200
C	-2.20571900	-3.41429300	2.75290000
C	-3.47415800	-3.40926200	2.18131600
C	-3.62831100	-3.38314800	0.79929200
H	-4.62780400	-3.36898900	0.35784300
C	-2.51625700	-3.35609200	-0.04911800
C	1.49514700	-3.93389900	-1.67850700
C	0.43906300	-4.38782000	-0.95244800
C	4.56973700	-0.09184800	-3.00899300
H	5.35344400	0.55050800	-3.41846500
C	3.39515700	-0.29056800	-3.72830900
H	3.25774700	0.19297900	-4.69895600
C	2.37730700	-1.11655400	-3.23465200

C	0.30937900	3.31573100	-2.54942800	H	-2.24911700	-2.37813600	-1.96607300
H	1.00809900	4.02737300	-2.08327400	C	3.90663300	-2.17545500	0.11094200
H	0.75090100	2.31103200	-2.41938400	H	3.16720700	-1.77203100	0.82358400
H	0.28312700	3.51915100	-3.62658600	H	3.73964900	-3.26276400	0.06615900
C	3.90648400	2.17611900	-0.11054900	H	4.90342200	-2.00787500	0.53639600
H	3.16729700	1.77268200	-0.82342000	C	1.11128900	-1.34598200	-3.99185200
H	3.73948000	3.26342400	-0.06583800	H	0.86916000	-2.41517900	-4.08453800
H	4.90339200	2.00855200	-0.53573700	H	0.23768600	-0.88019300	-3.50083500
C	1.11054900	1.34704200	3.99186100	H	1.16642000	-0.92655100	-5.00301900
H	0.23650300	0.88356800	3.49949200	C	-2.65972400	3.30805100	1.53490300
H	1.16451600	0.92562700	5.00226200	H	-2.24995500	2.37772500	1.96589700
H	0.87007500	2.41645900	4.08644200	H	-2.14254700	4.14251400	2.03312600
C	0.31001600	-3.31601500	2.54923300	H	-3.71350200	3.34514400	1.83368200
H	1.00895100	-4.02719600	2.08270600	H	0.01604300	-5.38161600	-0.84447500
H	0.75124300	-2.31112000	2.41968700	H	2.19025600	-4.44761000	-2.33546300
H	0.28382100	-3.51996300	3.62629300	H	-2.09554600	-3.40411000	3.83915000
C	-2.65905100	-3.30839900	-1.53511600	H	-4.35418200	-3.40287600	2.82697300
H	-2.14196600	-4.14292600	-2.03333400	Ag	-1.20543900	0.20464700	-1.44546300
H	-3.71282800	-3.34532900	-1.83392500	Ag	-1.20525400	-0.20517200	1.44566800

B_2IDip_2…3AgCl compound

B	-0.05793900	0.78482600	0.08936500	N	-1.07902300	3.17488700	0.02352800
B	0.03907000	-0.75860600	0.05914200	C	0.70046400	4.45479600	0.22573500
N	1.07588500	3.13085100	0.25733400	H	1.43118200	5.25238300	0.31511500
C	-0.02143400	2.32287500	0.12857400	Cl	1.15432500	0.27181600	-4.28468800
Cl	2.10352300	-0.18803900	4.07396900	C	3.24860300	2.30508200	-0.53550100

C	2.40902000	2.66827200	0.52805400
N	1.27725700	-3.03641500	-0.11339200
C	-0.65070700	4.48409400	0.07434900
H	-1.35041300	5.31066600	0.00112900
N	-0.63121200	-3.13314200	0.91363000
C	4.50623800	1.78939300	-0.19636200
H	5.18079600	1.48701300	-1.00195200
C	4.89790600	1.66087800	1.13181100
H	5.87853800	1.24009900	1.36966300
C	4.05600000	2.07061300	2.16287800
H	4.35785100	1.95794600	3.20605000
C	2.79211400	2.59489000	1.88088800
C	-2.46331100	2.80127300	-0.07701200
C	-4.49263000	2.09312500	0.96469700
H	-5.04291900	1.76075300	1.84891700
C	-3.13283400	2.39522500	1.09033000
C	-5.14030400	2.20361300	-0.26135500
H	-6.19839800	1.94695600	-0.33998200
C	-4.44243100	2.59509400	-1.39866900
H	-4.94476000	2.62101000	-2.36748500
C	-3.08033000	2.89558100	-1.33537900
C	0.21252900	-2.27618800	0.26890000
C	-1.94412800	-2.78434700	1.38877400
C	-4.28807600	-2.61744000	0.92887300
H	-5.12991500	-2.74487600	0.24600900
C	-3.01831600	-3.02280200	0.51207800
C	2.40166600	-2.55157000	-0.86674500
C	2.29119800	-2.56901200	-2.26948200
C	3.36745800	-2.06375400	-3.00232300
C	4.50081800	-1.57790000	-2.35453900
H	5.32951700	-1.17901400	-2.94489300
C	4.58255700	-1.58910600	-0.96689200
H	5.47652600	-1.20822900	-0.46487100
C	3.52934500	-2.07570100	-0.18165500
C	-0.09383200	-4.40115900	0.93655700
C	1.10324100	-4.34093000	0.29172900
C	-4.46681700	-2.00942400	2.16912800
H	-5.46496400	-1.68446500	2.47266000
C	-3.38821800	-1.81803200	3.02512000
H	-3.53911600	-1.35762300	4.00569700
C	-2.09341300	-2.20963800	2.65940200
C	1.88564700	3.07290400	2.97161500
H	1.83559400	4.17402400	2.99810700
H	0.85169500	2.71326600	2.84421400
H	2.22562600	2.71670600	3.95027300
C	-2.41546900	2.25382100	2.39444700
H	-1.76888100	1.35683000	2.40432200
H	-1.76297500	3.11289800	2.61213200
H	-3.12159700	2.15029000	3.22736700
C	-2.28135100	3.21300100	-2.55839000
H	-1.48568400	2.46481000	-2.71878900
H	-2.90978500	3.20629400	-3.45572000

H	-1.78360800	4.19340100	-2.50301400	H	0.01512400	-2.33981900	3.20394900
C	1.05391400	-3.07608000	-2.94086600	H	-0.85080300	-0.98875300	3.93798300
H	0.87355900	-4.14223200	-2.72818800	H	-1.11883500	-2.62083500	4.52906100
H	0.15386600	-2.52989400	-2.60861000	C	2.87517100	2.50592400	-1.96812600
H	1.11144500	-2.94261200	-4.02664800	H	3.08339100	1.61725200	-2.58145800
C	3.63710100	-2.07124000	1.30844600	H	1.81550400	2.75414100	-2.11638900
H	2.72648100	-2.40810300	1.82161300	H	3.46020600	3.33022300	-2.40647400
H	4.46012500	-2.71735700	1.65009500	Cl	-3.98617600	-0.65658600	-1.94413900
H	3.85836100	-1.06272600	1.69126600	H	3.28887200	-2.01870900	-4.08974100
C	-2.79393500	-3.65434300	-0.82400000	H	1.84914600	-5.10237500	0.08719600
H	-2.06005300	-3.08831300	-1.42031600	H	-0.61417400	-5.22765900	1.41010100
H	-2.41406900	-4.68489100	-0.73382400	Ag	-1.98340800	-0.17338200	-0.72551500
H	-3.71703100	-3.67266900	-1.41257200	Ag	1.04037100	0.00091200	1.93147200
C	-0.95683900	-2.03415100	3.61199900	Ag	0.65942900	0.11250700	-1.95259900

B_2IDip_2…AuCl

B	0.51872800	-0.62719200	0.00817600	N	-0.91794100	3.17403200	0.10893900
B	0.18786300	0.82918100	-0.03354400	C	2.18565700	-3.93180500	0.48068300
N	0.21384100	-3.03721200	0.89772700	H	3.06027700	-4.56274700	0.35499800
C	0.94868900	-2.04629000	0.29332500	N	1.22997800	3.12704700	0.46363100
N	2.16756100	-2.62025000	0.04024700	C	-3.48245300	-3.13223200	0.99720400
C	0.96277500	-4.18884300	1.01587700	H	-4.31101300	-3.44966200	0.36146900
H	0.55617400	-5.08654800	1.47174600	C	-3.72722100	-2.44582300	2.18143600
Cl	-3.57985000	-1.04208700	-1.79538600	H	-4.75700100	-2.26055600	2.49613900
C	-2.17442500	-3.36009100	0.56097200	C	-2.67146800	-1.97408100	2.95730400
C	-1.13276900	-2.87369200	1.36435900	H	-2.87091900	-1.42734900	3.88340800

C	-1.34566800	-2.17515000	2.56300400
C	3.23254100	-2.00318100	-0.68868300
C	5.45917900	-1.12044600	-0.72032800
H	6.36928200	-0.81947300	-0.19416000
C	4.38243700	-1.61862200	0.01827900
C	5.37065600	-0.98242100	-2.10300700
H	6.22123600	-0.58977700	-2.66612100
C	4.20120500	-1.33237800	-2.77171600
H	4.13372600	-1.21432600	-3.85639400
C	3.10435800	-1.86026400	-2.08082200
C	0.15853800	2.31636000	0.15686300
C	2.57764600	2.68370900	0.62853900
C	4.70309600	2.11393800	-0.31099500
H	5.34082000	1.94129300	-1.18152500
C	3.36207300	2.45469000	-0.51289200
C	-2.28225900	2.77279100	-0.06673400
C	-2.84922600	2.85884500	-1.34727100
C	-4.18430400	2.47417600	-1.48717500
C	-4.91068100	2.01222300	-0.39457900
C	-4.31822500	1.92362700	0.86101300
H	-4.88754500	1.53694600	1.71044300
C	-2.98611900	2.30070000	1.05259800
C	0.81978000	4.44023400	0.60790300
C	-0.51968800	4.46718500	0.38274500
C	5.22524200	1.98604000	0.97320900
H	6.27856600	1.72540200	1.10795800
C	4.41146500	2.17463500	2.08664600
H	4.81817900	2.04799800	3.09386400
C	3.06547200	2.52410200	1.93475600
C	-0.20161800	-1.61964800	3.34718500
H	0.60637100	-2.35366000	3.49047900
H	0.24692200	-0.75972900	2.81757700
H	-0.52522400	-1.27545600	4.33780800
C	4.42140800	-1.70693700	1.51042200
H	3.55520600	-1.19162900	1.95577400
H	4.38842000	-2.74555900	1.87479500
H	5.33104700	-1.24469000	1.91358500
C	1.84899200	-2.24779400	-2.79087800
H	1.04465100	-1.51447800	-2.60705700
H	2.00456100	-2.30885400	-3.87475700
H	1.45927300	-3.21766200	-2.44714900
C	-2.01407900	3.26850300	-2.51730400
H	-1.54737800	4.25628800	-2.38106700
H	-1.19189800	2.55058900	-2.67292200
H	-2.60528000	3.29875400	-3.44008400
C	-2.30316000	2.13381100	2.37106900
H	-1.70958100	3.01580700	2.65723900
H	-3.02336500	1.93217000	3.17403000
H	-1.60133000	1.28147900	2.32654300
C	2.76806400	2.54183700	-1.87978000
H	2.04724400	1.71898800	-2.03279300
H	2.20648600	3.47635900	-2.03177200

H	3.53762200	2.46941900	-2.65820900	H	-1.25644800	-3.36775000	-1.37948900
C	2.15503600	2.69353100	3.10904700	H	-1.35219000	-4.97405800	-0.63217500
H	1.76643600	3.72029200	3.19510600	H	-5.94432300	1.68799400	-0.53164900
H	1.27444700	2.03699100	3.02271400	H	-4.64313600	2.49643300	-2.47810600
H	2.66621700	2.45513300	4.04985700	H	-1.22960600	5.28873100	0.39100900
C	-1.88608500	-4.01732900	-0.74973900	H	1.52301600	5.23365300	0.84270300
H	-2.80872700	-4.20211100	-1.31104600	Au	-1.51835400	-0.33453000	-0.73763800

B_2IDip_2…2AuCl

B	-0.55396300	0.33127100	0.52726900	C	-4.46886300	-3.12729800	0.11587200
B	0.55372000	0.33168100	-0.52700200	H	-4.94117800	-3.94960100	-0.42512700
N	-2.58924200	0.02966800	2.12866700	C	-4.76272300	-1.81396300	-0.23689900
C	-1.43534100	0.63837600	1.74035100	H	-5.45172300	-1.60976800	-1.05938100
Cl	-2.29668300	-2.35573000	-2.71684900	C	-4.14320800	-0.74397700	0.41204900
N	-1.18243200	1.57398000	2.69925000	C	-0.14387100	2.56003100	2.63087700
C	-3.04239100	0.57163500	3.31467900	C	0.53059000	4.73508500	1.88895700
H	-3.94766600	0.20929800	3.79209600	H	0.32449000	5.66361000	1.34893800
Cl	2.29723700	-2.35660700	2.71558400	C	-0.43798100	3.73130800	1.90894600
C	-2.91373000	-2.36545500	1.81760800	C	1.74898000	4.55835800	2.54430300
C	-3.23290900	-1.05361200	1.43502100	H	2.49933200	5.35247300	2.51844400
N	2.58934000	0.03145500	-2.12826800	C	2.01454500	3.38151400	3.23368500
C	-2.16012900	1.54247100	3.67250800	H	2.97098800	3.25197600	3.74731800
H	-2.13630700	2.21493300	4.52431500	C	1.06647100	2.34848000	3.30486500
N	1.18208000	1.57554400	-2.69837000	C	1.43516900	0.63960700	-1.73984800
C	-3.55634800	-3.40008700	1.12934700	C	0.14326800	2.56133400	-2.62970800
H	-3.31841400	-4.43415800	1.39001200	C	-0.53169100	4.73599100	-1.88703900

H	-0.32582900	5.66436000	-1.34665600
C	0.43709100	3.73240700	-1.90732700
C	3.23320200	-1.05211900	-1.43526200
C	4.14349400	-0.74291500	-0.41214100
C	4.76344400	-1.81314400	0.23596500
C	4.47000900	-3.12633100	-0.11775800
C	3.55748500	-3.39869500	-1.13133400
H	3.31993200	-4.43265700	-1.39278100
C	2.91444900	-2.36377700	-1.81879400
C	2.15994600	1.54481200	-3.67149400
C	3.04249400	0.57413400	-3.31394800
C	-1.74998600	4.55927600	-2.54255000
H	-2.50046700	5.35326100	-2.51650800
C	-2.01525200	3.38264500	-3.23240000
H	-2.97160500	3.25312500	-3.74620600
C	-1.06699200	2.34980100	-3.30387200
C	-4.36786300	0.67013800	-0.01797600
H	-4.56021400	1.34935600	0.82649300
H	-3.47692200	1.05900300	-0.54320900
H	-5.21252900	0.74597100	-0.71328000
C	-1.73664600	3.86602900	1.18175000
H	-1.79042700	3.15198100	0.34155500
H	-2.60284400	3.65713300	1.82858400
H	-1.86342700	4.87335500	0.76724300
C	1.35961600	1.09778400	4.06715800
H	0.47496800	0.46642700	4.21884700
H	2.09188500	0.46288700	3.54214100
H	1.78831800	1.32647400	5.05295200
C	4.36767800	0.67099800	0.01879500
H	4.56091500	1.35064900	-0.82513500
H	3.47616700	1.05960000	0.54323000
H	5.21159900	0.74650500	0.71503400
C	1.90567000	-2.63298800	-2.88702800
H	2.13373300	-2.10260000	-3.82441500
H	1.84286800	-3.70290100	-3.11615900
H	0.89380900	-2.31122600	-2.58343700
C	1.73573500	3.86719800	-1.18010600
H	1.78954100	3.15313800	-0.33993700
H	2.60198000	3.65839800	-1.82691200
H	1.86243100	4.87451700	-0.76553600
C	-1.35984600	1.09938500	-4.06672000
H	-0.47506400	0.46827000	-4.21864800
H	-2.09198400	0.46411000	-3.54198300
H	-1.78859000	1.32838600	-5.05241700
C	-1.90500400	-2.63510800	2.88579200
H	-0.89327800	-2.31246500	2.58274000
H	-2.13362400	-2.10581500	3.82366200
H	-1.84162400	-3.70521700	3.11388000
H	3.94799800	0.21236600	-3.79136000
H	2.13605100	2.21769700	-4.52296400
H	5.45247300	-1.60931900	1.05851700
H	4.94268100	-3.94886300	0.42257700

Au	-1.13078500	-0.96144800	-1.14139200	Au	1.13083200	-0.96184600	1.14097100

B_2IDip_2…3AuCl

B	-0.09937100	0.73079200	0.31045700	C	-4.51745300	2.71237400	1.17717800
B	0.01198500	-0.77291800	-0.27549800	H	-5.20819600	2.41120300	1.96815000
N	1.18572700	2.85566100	1.16417700	C	-3.14555000	2.70155900	1.43349300
C	0.05237400	2.22801500	0.72975100	C	-5.00343100	3.08067800	-0.07336300
Cl	1.54767100	-1.46105300	3.90181500	H	-6.07917100	3.07002000	-0.25864400
N	-0.89217300	3.20404200	0.67446300	C	-4.13261000	3.42750000	-1.09987500
C	0.94712900	4.19685600	1.36091700	H	-4.52370700	3.68152700	-2.08784600
H	1.73129900	4.86362400	1.70558200	C	-2.74902700	3.42782400	-0.90108000
Cl	1.43661200	1.69942600	-3.79840500	C	0.29450600	-2.26374700	-0.65928800
C	3.45707700	2.19245100	0.51432500	C	-1.81640000	-3.37285000	0.12435600
C	2.44663700	2.24319600	1.48504900	C	-4.19060200	-3.30808700	-0.14180000
N	1.43553500	-2.75964400	-1.21886500	H	-5.07045200	-3.16900100	-0.77203900
C	-0.35702700	4.41767200	1.05264600	C	-2.92542500	-3.24213700	-0.72725700
H	-0.96322200	5.31782400	1.06730100	C	2.61106000	-2.01784500	-1.58810900
N	-0.50932400	-3.34838300	-0.47723300	C	2.70047600	-1.56009800	-2.91519400
C	4.66408600	1.59041600	0.89617700	C	3.84360400	-0.83988700	-3.26898200
H	5.47548400	1.54103000	0.16519300	C	4.86266200	-0.62664900	-2.34428000
C	4.84002800	1.07112100	2.17351400	H	5.75081800	-0.06120000	-2.63808400
H	5.78493500	0.58938800	2.43875000	C	4.76010300	-1.12988100	-1.05242700
C	3.82881800	1.17717500	3.12596900	H	5.57260200	-0.98078400	-0.33645600
H	3.96626600	0.77079800	4.13021200	C	3.62456100	-1.83648500	-0.63510600
C	2.61583700	1.79072000	2.80766900	C	0.11767500	-4.49277600	-0.91759400
C	-2.29546500	3.07182100	0.37776000	C	1.33884300	-4.12334300	-1.38395500

C	-4.32987200	-3.49903800	1.22979400
H	-5.32820700	-3.53126400	1.67199100
C	-3.21072800	-3.64304400	2.04129800
H	-3.32768800	-3.80173700	3.11653300
C	-1.91740900	-3.59760900	1.50554400
C	1.55145100	1.99321700	3.83904900
H	1.47028500	3.05557900	4.12350000
H	0.55657200	1.68128900	3.48517000
H	1.76206300	1.40892100	4.74134700
C	-2.58468400	2.27293700	2.75117200
H	-2.01816000	1.32948100	2.65399000
H	-1.88948100	3.01519600	3.17438600
H	-3.37837500	2.10048900	3.48723800
C	-1.79343700	3.72374100	-2.01024200
H	-1.31499800	2.79892600	-2.37738800
H	-2.30261000	4.18058700	-2.86666000
H	-0.97307400	4.39260000	-1.70991200
C	1.61894900	-1.83704700	-3.91037200
H	1.69707700	-2.86019000	-4.31385200
H	0.61221300	-1.74347400	-3.47458000
H	1.67328600	-1.13430900	-4.74933300
C	3.54702200	-2.36411100	0.76127100
H	2.63740000	-2.94266700	0.96809500
H	4.40727500	-3.01300800	0.98341600
H	3.57526900	-1.54960700	1.50249800
C	-2.74636900	-3.02301100	-2.19529400
H	-2.08071400	-2.16911500	-2.40222400
H	-2.30223600	-3.90150900	-2.69166800
H	-3.70331200	-2.80109700	-2.68038100
C	-0.73044900	-3.82416900	2.38555700
H	0.23222000	-3.67075600	1.88073100
H	-0.73140800	-3.15360500	3.25606900
H	-0.72900300	-4.85168300	2.78174100
C	3.30981600	2.77073400	-0.85490000
H	3.38269000	1.99833200	-1.63580600
H	2.35123000	3.28046300	-1.01709100
H	4.11106900	3.49711700	-1.05748900
Cl	-4.34068700	-0.09892000	-1.03654300
Au	0.70665900	-0.65608200	1.80930500
Au	0.73918600	0.71112900	-1.73259500
Au	-2.04186800	-0.02742000	-0.34457000
H	3.91257700	-0.42414400	-4.27607600
H	2.15251300	-4.69785300	-1.81514100
H	-0.36854900	-5.46086400	-0.84985800

Table S4 EDA results of $B_2IDip_2\cdots nMCl$(n=1, 2, 3; M=Cu, Ag, and Au) interactions(in kcal/mol)

	CuCl	AgCl	AuCl	2CuCl	2AgCl	2AuCl	3CuCl	3AgCl	3AuCl
ΔE	-96.9	-81.0	-110.3	-182.47	-158.8	-200.2	-254.0	-229.4	-300.7
ΔE_{Pauli}	134.7	145.9	232.9	321.8	302.8	471.8	581.0	481.3	799.6
ΔE_{elstat}	-153.4	-161.0	-241.2	-316.8	-311.2	-452.6	-514.0	-497.9	-751.9
ΔE_{orb}	-78.3	-66.0	-102.0	-187.4	-145.3	-219.4	-321.1	-212.8	-348.4
[a]ΔE_{elstat}%	66.2	70.9	70.3	62.8	68.2	67.4	61.6	70.1	68.3
[a]ΔE_{orb}%	33.8	29.1	29.7	37.2	31.8	32.6	38.4	29.9	31.7

[a]$\Delta E_{elstat}\% = \Delta E_{elstat}/(\Delta E_{elstat}+\Delta E_{orb})$; $\Delta \boldsymbol{E}_{orb}\% = \Delta E_{orb}/(\Delta E_{elstat}+\Delta E_{orb})$

Table S5 Natural population analysis charges and Wiberg bond indexes of the studied complexes

□	B_2IDip_2	CuCl	AgCl	AuCl	2CuCl	2AgCl	2AuCl	3CuCl	3AgCl	3AuCl
WBI_{B-B}	1.97	1.96	1.99	1.85	1.80	1.92	1.70	1.74	1.93	1.52
WBI_{B1-M1}		0.36	0.31	0.46	0.36	0.28	0.47	0.28	0.24	0.36
WBI_{B2-M1}		0.38	0.31	0.47	0.34	0.27	0.39	0.29	0.24	0.34
WBI_{B1-M2}					0.34	0.27	0.39	0.34	0.20	0.34
WBI_{B2-M2}					0.36	0.28	0.47	0.35	0.19	0.37
WBI_{B1-M3}								0.29	0.23	0.41
WBI_{B2-M3}		□	□	□	□	□	□	0.28	0.24	0.41
q(B1+B2)	-0.25	-0.54	-0.48	-0.40	-0.68	-0.61	-0.52	-0.89	-0.83	-0.65
Δq(B1+B2)		-0.29	-0.23	-0.15	-0.42	-0.36	-0.27	-0.64	-0.58	-0.40
Δq_{MCl1}		-0.08	-0.20	-0.29	-0.07	-0.15	-0.23	0.001	-0.11	-0.17
Δq_{MCl2}					-0.07	-0.15	-0.23	-0.08	-0.10	-0.17
Δq_{MCl3}								0.02	-0.11	-0.16
$Sum\Delta q_{(M+Cl)}$		-0.08	-0.20	-0.29	-0.13	-0.31	-0.46	-0.07	-0.32	-0.50
Average		-0.08	-0.20	-0.29	-0.07	-0.15	-0.23	-0.02	-0.11	-0.17

Table S6 A selection of NBO results for the studied complexes

Complexes	Donor NBO	δ_{donor}	[a]Acceptor NBO	δ_{acc}	Δ^2E (kcal/mol)	[b]Donor NBO	δ_{donor}	[b]Acceptor NBO	δ_{acc}	Δ^2E (kcal/mol)
B_2IDip_2…CuCl	BD(B1-B2)	1.6231	LP*Cu1	0.4233	109.43	LPCu1	1.8665	BD* (B1-B2)	0.0778	6.72
B_2IDip_2…2CuCl	BD(B1-B2)	1.5576	LP*Cu1	0.4165	47.56	LPCu1	1.8626	BD* (B1-B2)	0.1403	4.93
	BD(B1-B2)	1.5576	LP*Cu2	0.4164	48.42	LPCu2	1.8625	BD* (B1-B2)	0.1403	5.05
B_2IDip_2…3CuCl	BD(B1-B2)	1.6168	LP*Cu1	0.3761	32.77	LPCu1	1.8666	BD* (B1-B2)	0.2443	9.03
	BD(B1-B2)	1.5324	LP*Cu2	0.1894	49.45	LPCu2	1.8547	BD* (B1-B2)	0.2019	12.49
	BD(B1-B2)	1.6168	LP*Cu3	0.3589	58.71	LPCu3	1.8664	BD* (B1-B2)	0.2443	12.85
B_2IDip_2…AgCl	BD(B1-B2)	1.6242	LP*Ag1	0.4738	136.41	LPAg1	1.9169	BD* (B1-B2)	0.0700	6.99
B_2IDip_2…2AgCl	BD(B1-B2)	1.5373	LP*Ag1	0.4299	63.8	LPAg1	1.9137	BD* (B1-B2)	0.1263	6.26
	BD(B1-B2)	1.5373	LP*Ag2	0.4298	63.83	LPAg2	1.9138	BD* (B1-B2)	0.1263	6.25
B_2IDip_2…3AgCl	BD(B1-B2)	1.6249	LP*Ag1	0.3531	67.43	LPAg1	1.9245	BD* (B1-B2)	0.2059	6.13
	BD(B1-B2)	1.6249	LP*Ag2	0.3806	78.14	LPAg2	1.9119	BD* (B1-B2)	0.2059	9.06
	BD(B1-B2)	1.7387	LP*Ag3	0.3764	63.64	LPAg3	1.9101	BD* (B1-B2)	0.1080	7.77
B_2IDip_2…AuCl	BD(B1-B2)	1.5330	LP*Au1	0.6930	301.26	LPAu1	1.8658	BD* (B1-B2)	0.0790	8.77
B_2IDip_2…2AuCl	BD(B1-B2)	1.5035	LP*Au1	0.6480	215.18	LPAu1	1.8584	BD* (B1-B2)	0.1726	10.27
	BD(B1-B2)	1.5035	LP*Au2	0.6480	215.16	LPAu2	1.8585	BD* (B1-B2)	0.1726	10.26
B_2IDip_2…3AuCl	BD(B1-B2)	1.5281	LP*Au1	0.6024	375.59	LPAu1	1.8696	BD* (B1-B2)	0.2648	14.54
	BD(B1-B2)	1.5281	LP*Au2	0.5991	347.58	LPAu2	1.8648	BD* (B1-B2)	0.2648	14.73
	BD(B1-B2)	1.5773	LP*Au3	0.6145	340.07	LPAu3	1.8390	BD* (B1-B2)	0.2033	21.93

Table S7 Topological parameters at the BCP of the π(B≡B)···M interaction and B≡B, B-C bonds

	BCP	CuCl	AgCl	AuCl	2CuCl	2AgCl	2AuCl	3CuCl	3AgCl	3AuCl
M-B	ρ	0.087	0.079	0.098	0.084	0.076	0.096	0.082	0.077	0.096
	$\nabla^2\rho$	0.189	0.121	0.087	0.179	0.116	0.069	0.179	0.116	0.043
	H_c	-0.023	-0.025	-0.038	-0.023	-0.024	-0.038	-0.022	-0.024	-0.040
	$-G_c/V_c$	0.751	0.688	0.611	0.749	0.690	0.596	0.755	0.690	0.560
	DI	0.594	0.559	0.615	0.521	0.473	0.621	0.452	0.454	0.605
B-B	ρ	0.172	0.174	0.172	0.166	0.168	0.161	0.150	0.145	0.129
	$\nabla^2\rho$	-0.299	-0.320	-0.340	-0.279	-0.301	-0.263	-0.189	-0.161	-0.087
	H_c	-0.169	-0.172	-0.151	-0.133	-0.134	-0.124	-0.109	-0.104	-0.081
	$-G_c/V_c$	0.358	0.349	0.304	0.322	0.305	0.319	0.362	0.380	0.422
	DI	1.357	1.324	1.268	1.278	1.249	1.046	1.136	1.085	0.725
B-C	ρ	0.181	0.181	0.180	0.177	0.177	0.175	0.172	0.174	0.167
	$\nabla^2\rho$	0.244	0.220	0.211	0.218	0.187	0.179	0.182	0.145	0.121
	H_c	-0.175	-0.172	-0.176	-0.171	-0.173	-0.170	-0.166	-0.170	-0.163
	$-G_c/V_c$	0.574	0.349	0.565	0.569	0.559	0.558	0.560	0.548	0.543
	DI	0.764	0.748	0.711	0.709	0.678	0.643	0.699	0.665	0.600