Regium–π vs Cation–π Interactions in M_2 and MCl (M = Cu, Ag and Au) Complexes with Small Aromatic Systems: An ab Initio Study

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Electronic Supporting Information

Cartesian Coordinates

10.

C	-0.7019720	-1.2158685	-0.4271887
C	-1.4039119	0.0000000	-0.4272853
C	-0.7019720	1.2158685	-0.4271887
C	0.7019720	1.2158685	-0.4271887
C	1.4039119	0.0000000	-0.4272853
C	0.7019720	-1.2158685	-0.4271887
H	-1.2432670	-2.1533868	-0.4045879
H	-2.4864803	0.0000000	-0.4047802
H	-1.2432670	2.1533868	-0.4045879
H	1.2432670	2.1533868	-0.4045879
H	2.4864803	0.0000000	-0.4047802
H	1.2432670	-2.1533868	-0.4045879
Cu	0.0000000	0.0000000	1.3529492
Cu	0.0000000	0.0000000	3.6382883

11.

C	-0.6989126	-1.2105385	-0.5152489
C	-1.3978420	0.0000000	-0.5152797

C	-0.6989126	1.2105385	-0.5152489
C	0.6989126	1.2105385	-0.5152489
C	1.3978420	0.0000000	-0.5152797
C	0.6989126	-1.2105385	-0.5152489
H	-1.2406260	-2.1488611	-0.5269202
H	-2.4813078	0.0000000	-0.5269990
H	-1.2406260	2.1488611	-0.5269202
H	1.2406260	2.1488611	-0.5269202
H	2.4813078	0.0000000	-0.5269990
H	1.2406260	-2.1488611	-0.5269202
Ag	0.0000000	0.0000000	1.8658959
Ag	0.0000000	0.0000000	4.3873381

12.

C	-0.7005489	-1.2134243	-0.4959957
C	-1.4010203	0.0000000	-0.4957456
C	-0.7005489	1.2134243	-0.4959957
C	0.7005489	1.2134243	-0.4959957
C	1.4010203	0.0000000	-0.4957456
C	0.7005489	-1.2134243	-0.4959957
H	-1.2422920	-2.1517126	-0.4970202
H	-2.4844821	0.0000000	-0.4964625
H	-1.2422920	2.1517126	-0.4970202
H	1.2422920	2.1517126	-0.4970202
H	2.4844821	0.0000000	-0.4964625
H	1.2422920	-2.1517126	-0.4970202
Au	0.0000000	0.0000000	1.7479352

Au	0.0000000	0.0000000	4.2085446

13.

C	0.7081874	1.2266166	-0.4263012
C	0.7081874	-1.2266166	-0.4263012
C	-1.4163748	0.0000000	-0.4263012
H	1.2488846	2.1631316	-0.4190719
H	1.2488846	-2.1631316	-0.4190719
H	-2.4977692	0.0000000	-0.4190719
Cu	0.0000000	0.0000000	1.4240166
Cu	-0.0000000	0.0000000	3.6976845
C	-0.6880254	-1.1916949	-0.4234588
C	1.3760508	0.0000000	-0.4234588
C	-0.6880254	1.1916949	-0.4234588
F	2.7079793	0.0000000	-0.4384018
F	-1.3539896	-2.3451788	-0.4384018
F	-1.3539896	2.3451788	-0.4384018

14.

C	0.7048174	1.2207796	-0.5393040
C	0.7048174	-1.2207796	-0.5393040
C	-1.4096349	0.0000000	-0.5393040
H	1.2455470	2.1573506	-0.5529164
H	1.2455470	-2.1573506	-0.5529164
H	-2.4910940	0.0000000	-0.5529164
Ag	0.0000000	0.0000000	2.0318201
Ag	0.0000000	0.0000000	4.5482841

C	-0.6839184	-1.1845814	-0.5459258
C	1.3678367	0.0000000	-0.5459258
C	-0.6839184	1.1845814	-0.5459258
F	2.7039121	0.0000000	-0.5552218
F	-1.3519561	-2.3416566	-0.5552218
F	-1.3519561	2.3416566	-0.5552218

15.

C	0.7061600	1.2231050	-0.5104429
C	0.7061600	-1.2231050	-0.5104429
C	-1.4123200	0.0000000	-0.5104429
H	1.2470017	2.1598702	-0.5147148
H	1.2470017	-2.1598702	-0.5147148
H	-2.4940033	0.0000000	-0.5147148
Au	0.0000000	0.0000000	1.8624562
Au	-0.0000000	0.0000000	4.3170888
C	-0.6855231	-1.1873608	-0.5125540
C	1.3710461	0.0000000	-0.5125540
C	-0.6855231	1.1873608	-0.5125540
F	2.7050355	0.0000000	-0.5221366
F	-1.3525178	-2.3426295	-0.5221366
F	-1.3525178	2.3426295	-0.5221366

16.

C	1.214384	0.701125	-0.405504
C	1.214384	-0.701125	-0.405504

C	-0.000000	-1.402250	-0.405504
C	-1.214384	-0.701125	-0.405504
C	-1.214384	0.701125	-0.405504
C	0.000000	1.402250	-0.405504
F	2.358907	1.361916	-0.432354
F	2.358907	-1.361916	-0.432354
F	0.000000	-2.723831	-0.432354
F	-2.358907	-1.361916	-0.432354
F	-2.358907	1.361916	-0.432354
F	0.000000	2.723831	-0.432354
Cu	-0.000000	-0.000000	1.379302
Cu	0.000000	0.000000	3.647848

17.

C	1.2056346	0.6960734	-0.5640319
C	1.2056346	-0.6960734	-0.5640319
C	0.0000000	-1.3921469	-0.5640319
C	-1.2056346	-0.6960734	-0.5640319
C	-1.2056346	0.6960734	-0.5640319
C	0.0000000	1.3921469	-0.5640319
F	2.3533398	1.3587013	-0.5584564
F	2.3533398	-1.3587013	-0.5584564
F	-0.0000000	-2.7174027	-0.5584564
F	-2.3533398	-1.3587013	-0.5584564
F	-2.3533398	1.3587013	-0.5584564
F	0.0000000	2.7174027	-0.5584564
Ag	0.0000000	-0.0000000	2.1102719

Ag	0.0000000	0.0000000	4.6246589

18.

C	1.2080082	0.6974438	-0.5270316
C	1.2080082	-0.6974438	-0.5270316
C	0.0000000	-1.3948877	-0.5270316
C	-1.2080082	-0.6974438	-0.5270316
C	-1.2080082	0.6974438	-0.5270316
C	0.0000000	1.3948877	-0.5270316
F	2.3542052	1.3592010	-0.5223590
F	2.3542052	-1.3592010	-0.5223590
F	0.0000000	-2.7184020	-0.5223590
F	-2.3542052	-1.3592010	-0.5223590
F	-2.3542052	1.3592010	-0.5223590
F	-0.0000000	2.7184020	-0.5223590
Au	-0.0000000	0.0000000	1.9223348
Au	0.0000000	0.0000000	4.3740100

19.

C	-0.7023975	-1.2165848	-0.4130212
C	-1.4047973	0.0000000	-0.4130475
C	-0.7023975	1.2165848	-0.4130212
C	0.7023975	1.2165848	-0.4130212
C	1.4047973	0.0000000	-0.4130475
C	0.7023975	-1.2165848	-0.4130212
H	-1.2436412	-2.1540574	-0.3891007
H	-2.4872952	0.0000000	-0.3891499

H	-1.2436412	2.1540574	-0.3891007
H	1.2436412	2.1540574	-0.3891007
H	2.4872952	0.0000000	-0.3891499
H	1.2436412	-2.1540574	-0.3891007
Cu	0.0000000	0.0000000	1.3542840
Cl	0.0000000	0.0000000	3.4585985

20.

C	-0.7000330	-1.2124919	-0.4790537
C	-1.4000674	0.0000000	-0.4790597
C	-0.7000330	1.2124919	-0.4790537
C	0.7000330	1.2124919	-0.4790537
C	1.4000674	0.0000000	-0.4790597
C	0.7000330	-1.2124919	-0.4790537
H	-1.2416716	-2.1506417	-0.4866935
H	-2.4833480	0.0000000	-0.4867071
H	-1.2416716	2.1506417	-0.4866935
H	1.2416716	2.1506417	-0.4866935
H	2.4833480	0.0000000	-0.4867071
H	1.2416716	-2.1506417	-0.4866935
Ag	0.0000000	0.0000000	1.7606854
Cl	0.0000000	0.0000000	4.0338374

21.

C	-0.7007395	-1.2137168	-0.4800663
C	-1.4014793	0.0000000	-0.4800575

C	-0.7007395	1.2137168	-0.4800663
C	0.7007395	1.2137168	-0.4800663
C	1.4014793	0.0000000	-0.4800575
C	0.7007395	-1.2137168	-0.4800663
H	-1.2423571	-2.1518240	-0.4735687
H	-2.4847129	0.0000000	-0.4735523
H	-1.2423571	2.1518240	-0.4735687
H	1.2423571	2.1518240	-0.4735687
H	2.4847129	0.0000000	-0.4735523
H	1.2423571	-2.1518240	-0.4735687
Au	0.0000000	0.0000000	1.7498126
Cl	0.0000000	0.0000000	3.9719472

22.

C	0.7086103	1.2273490	-0.4093706
C	0.7086103	-1.2273490	-0.4093706
C	-1.4172206	0.0000000	-0.4093706
H	1.2494448	2.1641019	-0.4006601
H	1.2494448	-2.1641019	-0.4006601
H	-2.4988896	0.0000000	-0.4006601
Cu	-0.0000000	0.0000000	1.4199060
C	-0.6889631	-1.1933191	-0.4086808
C	1.3779262	0.0000000	-0.4086808
C	-0.6889631	1.1933191	-0.4086808
F	2.7071387	0.0000000	-0.4238357
F	-1.3535693	-2.3444509	-0.4238357
F	-1.3535693	2.3444509	-0.4238357

Cl	0.0000000	0.0000000	3.5077353

23.

C	0.7062226	1.2232134	-0.4869374
C	0.7062226	-1.2232134	-0.4869374
C	-1.4124452	0.0000000	-0.4869374
H	1.2471055	2.1600501	-0.5017866
H	1.2471055	-2.1600501	-0.5017866
H	-2.4942110	0.0000000	-0.5017866
Ag	-0.0000000	0.0000000	1.8590725
C	-0.6858907	-1.1879976	-0.4927739
C	1.3717814	0.0000000	-0.4927739
C	-0.6858907	1.1879976	-0.4927739
F	2.7033391	0.0000000	-0.5113672
F	-1.3516696	-2.3411603	-0.5113672
F	-1.3516696	2.3411603	-0.5113672
Cl	0.0000000	0.0000000	4.1195229

24.

C	0.7067552	1.2241359	-0.4861333
C	0.7067552	-1.2241359	-0.4861333
C	-1.4135104	0.0000000	-0.4861333
H	1.2476537	2.1609996	-0.4838126
H	1.2476537	-2.1609996	-0.4838126
H	-2.4953074	0.0000000	-0.4838126
Au	-0.0000000	0.0000000	1.8287704
C	-0.6865514	-1.1891419	-0.4883443

C	1.3731028	0.0000000	-0.4883443
C	-0.6865514	1.1891419	-0.4883443
F	2.7041604	0.0000000	-0.4970584
F	-1.3520802	-2.3418716	-0.4970584
F	-1.3520802	2.3418716	-0.4970584
Cl	0.0000000	0.0000000	4.0372752

25.

C	1.2153695	0.7016939	-0.3942638
C	1.2153695	-0.7016939	-0.3942638
C	0.0000000	-1.4033878	-0.3942638
C	-1.2153695	-0.7016939	-0.3942638
C	-1.2153695	0.7016939	-0.3942638
C	0.0000000	1.4033878	-0.3942638
F	2.3573266	1.3610031	-0.4251900
F	2.3573266	-1.3610031	-0.4251900
F	0.0000000	-2.7220062	-0.4251900
F	-2.3573266	-1.3610031	-0.4251900
F	-2.3573266	1.3610031	-0.4251900
F	0.0000000	2.7220062	-0.4251900
Cl	0.0000000	0.0000000	3.4978705
Cu	-0.0000000	-0.0000000	1.4188523

26.

C	1.2094353	0.6982678	-0.4987572
C	1.2094353	-0.6982678	-0.4987572

C	0.0000000	-1.3965356	-0.4987572
C	-1.2094353	-0.6982678	-0.4987572
C	-1.2094353	0.6982678	-0.4987572
C	0.0000000	1.3965356	-0.4987572
F	2.3535101	1.3587997	-0.5155001
F	2.3535101	-1.3587997	-0.5155001
F	-0.0000000	-2.7175994	-0.5155001
F	-2.3535101	-1.3587997	-0.5155001
F	-2.3535101	1.3587997	-0.5155001
F	-0.0000000	2.7175994	-0.5155001
Ag	0.0000000	-0.0000000	1.9175260
Cl	0.0000000	0.0000000	4.1680174

27.

C	1.2102427	0.6987340	-0.4939298
C	1.2102427	-0.6987340	-0.4939298
C	0.0000000	-1.3974679	-0.4939298
C	-1.2102427	-0.6987340	-0.4939298
C	-1.2102427	0.6987340	-0.4939298
C	0.0000000	1.3974679	-0.4939298
F	2.3539636	1.3590615	-0.4947395
F	2.3539636	-1.3590615	-0.4947395
F	0.0000000	-2.7181231	-0.4947395
F	-2.3539636	-1.3590615	-0.4947395
F	-2.3539636	1.3590615	-0.4947395
F	0.0000000	2.7181231	-0.4947395
Au	-0.0000000	0.0000000	1.8663257

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Cl     0.0000000    -0.0000000     4.0656904
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