

Supporting Information for

“Unveiling the Nature of Ligand-Modulated

Argentophilic Interactions: A Theoretical Study of

Intra- and Intermolecular Silver Complexes”

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Table S1. The T1 diagnostic values of intramolecular model **1** and intermolecular **1b** calculated by using DLPNO-CCSD/def2-TZVP.

Compound	1	1b
T1 value	0.012	0.012

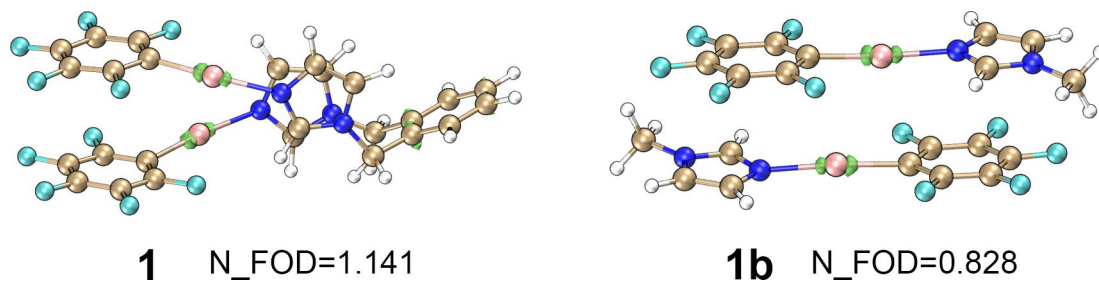


Figure S1. The Fractional Occupation Number Weighted Density (FOD) analysis (PBE0-D3(BJ)/def2-TZVP in 10000 K) at $\sigma=0.005$ e Bohr⁻³. No apparently visible FOD indicates that the electronic structure is of single-reference nature and common (double) hybrid density functionals should provide very reasonable results.

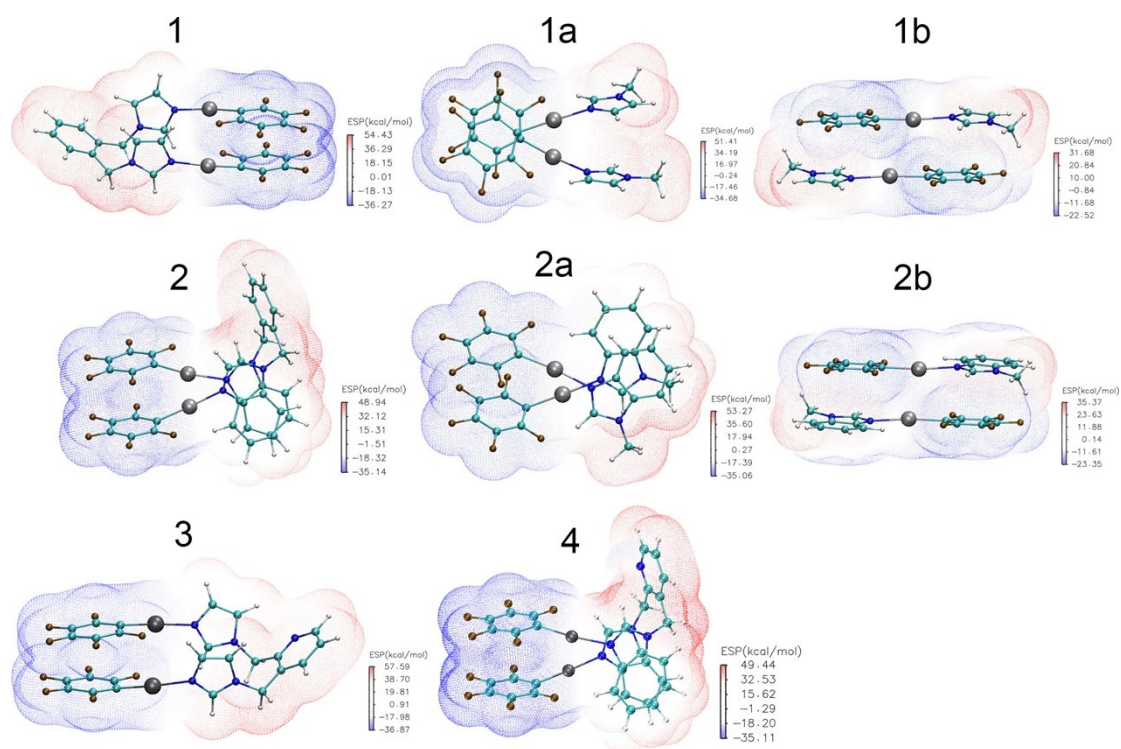


Figure S2. Electrostatic potential (ESP) mapped van der Waals surface analysis for inter- and intramolecular argentophilic complexes.

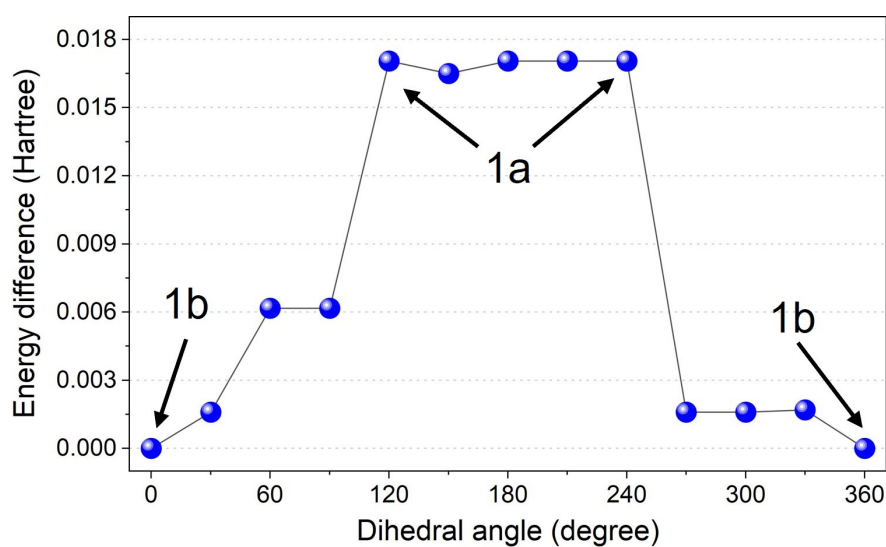


Figure S3. Relaxed scan of potential energy curve (PEC) from configuration **1b** to **1a** to **1b** with the dihedral angle γ of N-Ag-Ag'-C' as the reaction coordinate, the displacement is 30°, Y axis represents the energy difference of PEC structures with **1b**.

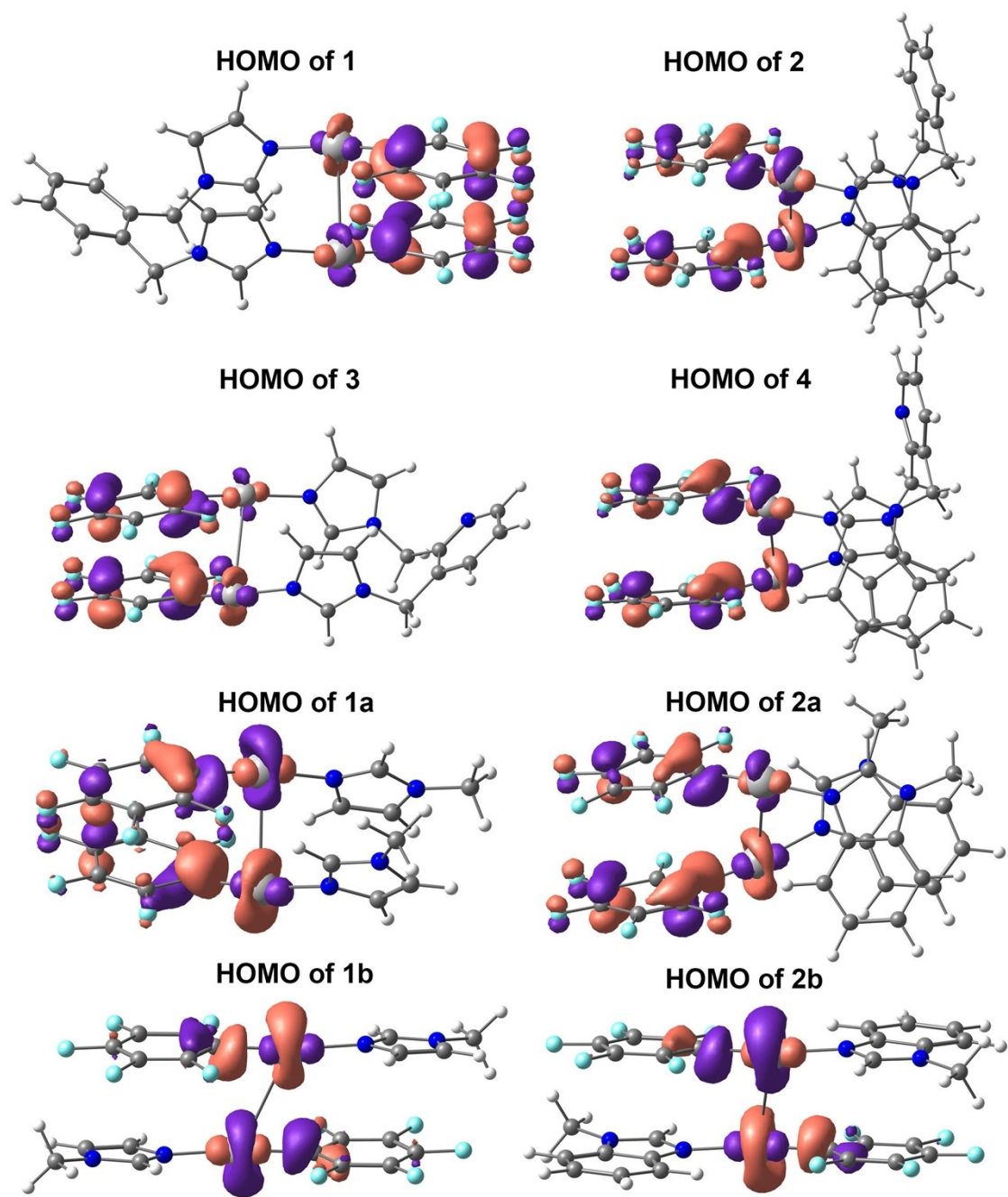


Figure S4. The Highest Occupied Molecular Orbitals (HOMOs) of inter- and intramolecular argentophilic complexes.

Table S2. The atomic oxidation states of inter- and intramolecular argentophilic complexes calculated by mLOBA approach based on the wavefunction of PBE0-D3(BJ)/def2-TZVP.

1	2	3	4	1a	1b	2a	2b
1(Ag):1	1(Ag):1	1(Ag):1	1(Ag):1	1(Ag):1	1(Ag):1	1(Ag):1	1(Ag):1
2(Ag):1	2(Ag):1	2(F):-1	2(F):-1	2(Ag):1	2(Ag):1	2(Ag):1	2(Ag):1
3(F):-1	3(F):-1	3(F):-1	3(F):-1	3(F):-1	3(F):-1	3(F):-1	3(F):-1
4(F):-1	4(F):-1	4(F):-1	4(F):-1	4(F):-1	4(F):-1	4(F):-1	4(F):-1
5(F):-1	5(F):-1	5(F):-1	5(F):-1	5(F):-1	5(F):-1	5(F):-1	5(F):-1
6(F):-1	6(F):-1	6(F):-1	6(F):-1	6(F):-1	6(F):-1	6(F):-1	6(F):-1
7(F):-1	7(F):-1	7(N):-3	7(N):-3	7(F):-1	7(F):-1	7(F):-1	7(F):-1
8(F):-1	8(F):-1	8(N):-3	8(N):-3	8(F):-1	8(F):-1	8(F):-1	8(F):-1
9(F):-1	9(F):-1	9(C):2	9(C):2	9(F):-1	9(F):-1	9(F):-1	9(F):-1
10(F):-1	10(F):-1	10(H):1	10(H):1	10(F):-1	10(F):-1	10(F):-1	10(F):-1
11(F):-1	11(F):-1	11(C):-2	11(C):0	11(F):-1	11(F):-1	11(F):-1	11(F):-1
12(F):-1	12(F):-1	12(H):1	12(C):0	12(F):-1	12(F):-1	12(F):-1	12(F):-1
13(N):-3	13(N):-3	13(C):2	13(H):1	13(N):-3	13(N):-3	13(N):-3	13(N):-3
14(N):-3	14(N):-3	14(H):1	14(C):0	14(N):-3	14(N):-3	14(N):-3	14(N):-3
15(N):-3	15(N):-3	15(C):2	15(H):1	15(N):-3	15(N):-3	15(N):-3	15(N):-3
16(N):-3	16(N):-3	16(C):0	16(C):0	16(N):-3	16(N):-3	16(N):-3	16(N):-3
17(C):2	17(C):2	17(C):0	17(H):1	17(C):2	17(C):2	17(C):2	17(C):2
18(H):1	18(H):1	18(C):0	18(C):-2	18(H):1	18(H):1	18(H):1	18(H):1
19(C):-2	19(C):0	19(C):2	19(H):1	19(C):-2	19(C):-2	19(C):0	19(C):0
20(H):1	20(C):0	20(C):0	20(C):0	20(H):1	20(H):1	20(C):0	20(C):0
21(C):2	21(H):1	21(C):0	21(C):2	21(C):2	21(C):2	21(H):1	21(H):1
22(H):1	22(C):0	22(H):1	22(C):0	22(H):1	22(H):1	22(C):0	22(C):0
23(C):2	23(H):1	23(H):1	23(C):0	23(C):2	23(C):0	23(H):1	23(H):1
24(C):0	24(C):0	24(C):-2	24(C):0	24(C):0	24(C):2	24(C):0	24(C):0
25(C):2	25(H):1	25(C):0	25(C):2	25(C):2	25(C):0	25(H):1	25(H):1
26(C):0	26(C):-2	26(H):1	26(C):0	26(C):-2	26(C):0	26(C):-2	26(C):-2

27(C):0	27(H):1	27(C):0	27(C):0	27(C):2	27(C):0	27(H):1	27(H):1
28(C):0	28(C):0	28(H):1	28(H):1	28(C):0	28(C):2	28(C):0	28(C):0
29(C):0	29(C):2	29(C):0	29(H):1	29(C):-2	29(C):-2	29(C):0	29(C):0
30(H):1	30(C):0	30(H):1	30(C):0	30(H):1	30(H):1	30(C):2	30(C):2
31(H):1	31(C):0	31(N):-3	31(N):-3	31(H):1	31(H):1	31(C):0	31(C):0
32(C):-2	32(C):0	32(C):0	32(C):0	32(H):1	32(H):1	32(C):0	32(C):0
33(C):0	33(C):2	33(Ag):1	33(H):1	33(H):1	33(H):1	33(C):0	33(C):0
34(H):1	34(C):0	34(F):-1	34(C):0	34(C):-2	34(C):-2	34(C):2	34(C):2
35(C):0	35(C):0	35(F):-1	35(H):1	35(H):1	35(H):1	35(C):2	35(C):-2
36(H):1	36(H):1	36(F):-1	36(C):0	36(H):1	36(H):1	36(H):1	36(H):1
37(C):0	37(H):1	37(F):-1	37(H):1	37(C):2	37(C):2	37(C):0	37(H):1
38(H):1	38(C):-2	38(F):-1	38(C):-2	38(H):1	38(H):1	38(C):0	38(C):-2
39(C):-2	39(C):-2	39(N):-3	39(Ag):1	39(C):-2	39(C):-2	39(H):1	39(H):1
40(H):1	40(H):1	40(N):-3	40(F):-1	40(H):1	40(H):1	40(C):0	40(H):1
41(C):-2	41(C):2	41(C):0	41(F):-1	41(C):2	41(C):2	41(H):1	41(C):2
42(C):0	42(H):1	42(H):1	42(F):-1	42(H):1	42(H):1	42(C):0	42(H):1
43(H):1	43(C):-2	43(H):1	43(F):-1	43(C):2	43(C):0	43(H):1	43(C):2
44(H):1	44(H):1	44(C):2	44(F):-1	44(C):0	44(C):2	44(C):-2	44(C):0
45(C):2	45(C):0	45(H):1	45(N):-3	45(C):2	45(C):0	45(H):1	45(H):1
46(H):1	46(H):1	46(C):-2	46(N):-3	46(C):0	46(C):0	46(C):0	46(C):0
47(C):-2	47(C):-2	47(H):1	47(C):0	47(C):0	47(C):0	47(C):2	47(H):1
48(H):1	48(C):0	48(C):2	48(H):1	48(C):0	48(C):2	48(C):0	48(C):0
49(C):2	49(H):1	49(H):1	49(H):1			49(C):2	49(H):1
50(H):1	50(H):1	50(C):2	50(C):2			50(C):-2	50(C):-2
51(C):2	51(C):2	51(C):0	51(H):1			51(C):0	51(H):1
52(C):0	52(H):1	52(C):2	52(C):0			52(C):2	52(C):-2
53(C):0	53(C):0	53(C):0	53(C):0			53(C):-2	53(C):0
54(C):0	54(C):0	54(C):0	54(H):1			54(H):1	54(C):2
55(C):2	55(H):1	55(C):0	55(C):0			55(H):1	55(C):0
56(C):0	56(C):0		56(H):1			56(H):1	56(C):0

57(H):1	57(C):0	57(C):-2	57(C):0
58(C):0	58(H):1	58(H):1	58(C):2
59(H):1	59(C):-2	59(H):1	59(H):1
60(C):-2	60(H):1	60(H):1	60(H):1
61(H):1	61(C):0		
62(C):0	62(C):2		
63(C):2	63(C):0		
64(C):0	64(C):2		
65(C):2	65(C):0		
66(C):0	66(C):0		
67(C):0	67(C):0		
68(C):0			

Table S3. The GKS-EDA, SAPT0, and DLPNO-CCSD(T) results of inter- and intramolecular argentophilic interactions with def2-TZVP basis, units in kcal/mol. Electron correlation energies of DLPNO-CCSD(T) are compared with ΔE^{disp} of SAPT0, and $\Delta E^{corr/disp}$ of GKS-EDA.

	Method	ΔE^{es}	ΔE^{exrep}	ΔE^{pol}	$\Delta E^{corr/disp}$	ΔE^{int}
1	PBE0-D3(BJ)	-14.34	38.78	-0.74	-30.13	-6.44
	ω B97x-D	-13.81	38.27	-1.14	-33.29	-9.99
1a	PBE0-D3(BJ)	-17.52	38.15	-5.02	-29.33	-13.72
	ω B97x-D	-17.10	37.60	-5.37	-30.69	-15.55
	SAPT0	-14.01	32.18	-5.23	-29.99	-17.05
	DLPNO-CCSD(T)/def2-TZVP/ <i>TightPNO</i>				-26.60	-14.95
	PBE0-D3(BJ)	-27.78	43.79	-7.69	-29.71	-21.40
1b	ω B97x-D	-27.35	43.23	-7.76	-32.27	-24.15
	BLYP-D3(BJ)	-30.42	48.19	-9.09	-32.58	-23.90
	M06-2X	-28.15	43.08	-5.60	-33.05	-23.72
	SAPT0	-27.74	39.09	-5.12	-34.73	-28.51
	DLPNO-CCSD(T)/def2-TZVP/ <i>TightPNO</i>				-30.61	-25.85
2	PBE0-D3(BJ)	-20.25	50.83	-2.80	-39.04	-11.28
	ω B97x-D	-19.68	50.19	-3.23	-42.63	-15.36
2a	PBE0-D3(BJ)	-19.87	46.10	-6.20	-37.65	-17.62
	ω B97x-D	-19.41	45.51	-6.48	-40.25	-20.63
	SAPT0	-17.12	40.78	-6.15	-41.06	-23.55
	DLPNO-CCSD(T)/def2-TZVP/ <i>TightPNO</i>				-37.16	-21.13
	PBE0-D3(BJ)	-28.15	48.28	-6.50	-37.69	-24.06
2b	ω B97x-D	-27.72	47.78	-6.28	-41.91	-28.13
	SAPT0	-29.15	45.79	-4.86	-46.14	-34.35
	DLPNO-CCSD(T)/def2-TZVP/ <i>TightPNO</i>				-41.62	-31.92
3	PBE0-D3(BJ)	-13.15	37.55	-3.50	-29.93	-9.04
	ω B97x-D	-12.62	37.13	-3.90	-32.90	-12.32
4	PBE0-D3(BJ)	-20.50	51.55	-6.22	-39.84	-14.99
	ω B97x-D	-19.92	50.99	-6.75	-43.29	-18.96

Table S4. The GKS-EDA results (PBE0-D3(BJ)/def2-TZVP) of potential energy curve (PEC) with dihedral angle γ of N-Ag-Ag'-C' as a reaction coordinate, units in kcal/mol.

γ (°)	ΔE^{es}	ΔE^{exrep}	ΔE^{pol}	$\Delta E^{corr/disp}$	ΔE^{int}
0	-27.78	43.79	-7.69	-29.71	-21.40
30	-25.66	39.63	-5.26	-29.63	-20.92
60	-21.47	31.73	-4.83	-25.06	-19.63
90	-21.48	31.75	-4.82	-25.08	-19.63
120	-17.52	38.14	-5.02	-29.33	-13.72
150	-17.52	38.15	-5.02	-29.32	-13.72
180	-17.52	38.15	-5.02	-29.32	-13.72
210	-17.53	38.16	-5.02	-29.33	-13.73
240	-17.53	38.16	-5.02	-29.33	-13.72
270	-25.67	39.65	-5.26	-29.65	-20.93
300	-25.66	39.62	-5.25	-29.65	-20.94
330	-26.75	41.27	-5.95	-29.56	-20.98

Geometric Structures

All in xyz format

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Optimized coordinates of **1** from PBE0-D3(BJ)/def2-SVP in G16

Ag	-0.18081500	0.57861800	-1.58058000
Ag	-0.20262100	-0.78563200	1.36400900
F	-1.02709800	-2.46733000	-1.31110200
F	-3.41256500	-3.63790900	-0.90849100
F	-5.68935300	-2.15460000	-0.95573600
F	-5.56194200	0.51500400	-1.41880600
F	-3.19605200	1.70279800	-1.86318900
F	-3.30174200	-1.58097800	1.93705200
F	-5.54291700	-0.12395200	1.69032900
F	-5.39746900	2.54688500	1.23543200
F	-2.97648400	3.75895800	1.00501100
F	-0.71554800	2.31558700	1.21579900
N	1.84081700	1.25839300	-1.39288500
N	3.78780000	1.40710000	-0.38613400
N	1.76005700	-1.57208000	1.00687600
N	3.95239000	-1.44810400	1.09398300

C	2.44520900	1.41766400	-0.23099400
H	1.94117100	1.53682300	0.72770200
C	4.04714000	1.24570500	-1.72856300
H	5.05740900	1.19654000	-2.12234200
C	2.82531500	1.15259900	-2.33915300
H	2.59820400	1.00824400	-3.39263900
C	-2.02388200	-0.34086300	-1.64527200
C	-2.13628300	-1.69897000	-1.39621100
C	-3.35105500	-2.33752000	-1.16877000
C	-4.51985500	-1.57911600	-1.18608900
C	-4.45119300	-0.21087700	-1.43941300
C	-3.20904200	0.37752000	-1.66633400
C	4.77378300	1.58619000	0.67422200
H	4.30251200	1.27002600	1.61469500
H	5.00269100	2.65884300	0.77222200
C	6.04735900	0.82949300	0.39476500
C	7.05434800	1.48535000	-0.31983800
H	6.90714600	2.53208000	-0.60059700
C	8.23340300	0.83717000	-0.67962500
H	9.00300000	1.37340800	-1.23878600
C	8.42043900	-0.49278000	-0.31844400
H	9.33701100	-1.01834700	-0.59436800
C	7.43410500	-1.15127400	0.41194300
H	7.59137200	-2.19037200	0.71327900
C	6.24800200	-0.51072700	0.78240900
C	5.27920200	-1.27068200	1.65414500
H	5.70659500	-2.25873300	1.88313200
H	5.14884400	-0.75512000	2.61868200
C	2.79403800	-1.27707700	1.76890500
H	2.74971400	-0.93851700	2.80325000
C	3.63139700	-1.88956700	-0.16886300
H	4.39144700	-2.09712800	-0.91691700
C	2.26200200	-1.95858500	-0.20945800
H	1.60332800	-2.24565100	-1.02684500
C	-1.92437700	0.31608300	1.62052600
C	-3.17805700	-0.26163100	1.74036400
C	-4.35820500	0.46866400	1.61749300
C	-4.28783300	1.83755800	1.36799800
C	-3.04439600	2.45694100	1.25578400
C	-1.89754700	1.68044200	1.38327100

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Optimized coordinates of **2** from PBE0-D3(BJ)/def2-SVP in G16

Ag	-0.41769100	-1.08521100	-0.98973400
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Ag	-0.35472100	0.67799400	1.55413400
F	-3.08757800	-0.43041900	-2.54565500
F	-5.66363800	-0.42850700	-1.79389300
F	-6.38515500	-1.43030200	0.62337900
F	-4.49363700	-2.42159300	2.30322800
F	-1.90971000	-2.39829900	1.59544600
F	-0.58075400	2.30227200	-1.12834500
F	-2.69200300	3.09442100	-2.58838200
F	-5.21580200	2.79159200	-1.62177900
F	-5.61144100	1.70195500	0.82743800
F	-3.51629400	0.92800900	2.32327700
N	1.62863400	-0.64117400	-1.43935400
N	3.55621800	0.44472600	-1.63028300
N	1.58982100	-0.11675000	2.00874300
N	3.75210000	0.00515000	1.49720800
C	2.22036900	0.52980500	-1.38311200
H	1.70961800	1.46944900	-1.16655600
C	2.60927600	-1.56310900	-1.75243400
C	2.52909500	-2.94499800	-1.93586900
H	1.57363900	-3.46154900	-1.82647600
C	3.70112500	-3.61689900	-2.25435400
H	3.67530200	-4.69755000	-2.40815200
C	4.92561100	-2.93626500	-2.38389900
H	5.82433700	-3.50071300	-2.64172800
C	5.02024100	-1.56050600	-2.20279200
H	5.97461000	-1.04382400	-2.32322600
C	3.83925500	-0.88789500	-1.88343400
C	-2.39676600	-1.45249300	-0.52601300
C	-3.39639800	-0.96121300	-1.35284400
C	-4.74146600	-0.94745700	-0.99265400
C	-5.11401300	-1.44425500	0.25458800
C	-4.14218100	-1.95683700	1.11089200
C	-2.81188400	-1.94118600	0.70166500
C	4.49988000	1.54261200	-1.71586100
H	4.29246900	2.12991000	-2.62346900
H	5.49182400	1.09038600	-1.86302000
C	4.53852500	2.47204800	-0.52611700
C	4.29891800	3.83132600	-0.74581000
H	4.02716400	4.16702100	-1.75005000
C	4.40413800	4.76402700	0.28371300
H	4.20457600	5.81899900	0.08499200
C	4.76886200	4.34314200	1.55821400
H	4.86492800	5.06350100	2.37320600
C	5.00443900	2.99018100	1.79198400

H	5.27948600	2.65442100	2.79578500
C	4.88349600	2.04277500	0.77182400
C	5.03460600	0.58746300	1.12969100
H	5.43259900	-0.00312900	0.29084000
H	5.74087600	0.47607100	1.96805300
C	2.61775700	0.67923100	1.81603700
H	2.58341200	1.76527100	1.87478200
C	2.05820100	-1.40333900	1.81140000
C	1.38583600	-2.62900100	1.83766500
H	0.31486100	-2.67484800	2.04073900
C	2.13451700	-3.76685900	1.56969000
H	1.64323900	-4.74201800	1.57955000
C	3.51114900	-3.69668500	1.28027000
H	4.05886200	-4.61819000	1.07245800
C	4.18876900	-2.48526900	1.23695900
H	5.25090900	-2.43784300	0.99254100
C	3.43288500	-1.34212900	1.49931900
C	-1.96877700	1.61587200	0.67308100
C	-1.81647700	2.17356300	-0.58491900
C	-2.88297000	2.58440700	-1.37731500
C	-4.17759100	2.42478900	-0.88766200
C	-4.37516500	1.87837900	0.37914700
C	-3.27036800	1.48644400	1.13166300

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Optimized coordinates of **3** from PBE0-D3(BJ)/def2-SVP in G16

Ag	-0.29970300	0.90168800	1.31549500
F	-3.33961500	1.98316000	1.56959000
F	-5.68059200	0.67340400	1.46626500
F	-5.73124300	-2.04033300	1.45144600
F	-3.40884900	-3.44602400	1.53195500
F	-1.04909700	-2.15463500	1.61289800
N	1.69334700	1.59873300	0.93543900
N	3.88480900	1.52608100	1.07404100
C	2.71629000	1.41039500	1.74504200
H	2.65682400	1.18931900	2.81002900
C	3.57985900	1.81742900	-0.23652200
H	4.34845000	1.95326500	-0.99222600
C	2.21110500	1.85633100	-0.30774000
H	1.56189300	2.03521800	-1.16272300
C	-2.10681300	-0.03542400	1.63319900
C	-3.31437100	0.64323600	1.59594400
C	-4.54472300	-0.00843500	1.54247600
C	-4.57380300	-1.40098900	1.51737200

C	-3.38033800	-2.11914500	1.56399200
C	-2.17909200	-1.41903100	1.61661300
C	5.20873600	1.43262200	1.66298900
H	5.09810300	0.92742200	2.63465200
H	5.58525900	2.44553200	1.87445300
C	6.20136200	0.71237000	0.78920000
C	7.29573900	1.41458200	0.27760200
H	7.41533700	2.47550000	0.51473800
C	8.22538000	0.76696500	-0.52676500
H	9.08757000	1.29621500	-0.93617500
C	8.02374500	-0.58425800	-0.79570900
H	8.72742000	-1.14062800	-1.42407800
N	6.99206300	-1.26756800	-0.31281400
C	6.09677900	-0.65150000	0.45710100
Ag	-0.01353900	-0.90169800	-1.41049300
F	-0.77672500	2.19481400	-1.67836400
F	-3.13981000	3.46318800	-1.60223200
F	-5.45592600	2.04078800	-1.51606000
F	-5.38641100	-0.66786900	-1.51727900
F	-3.03591400	-1.96496300	-1.62556900
N	1.96703000	-1.64940200	-1.07937900
N	3.93706100	-1.67474200	-0.10958800
C	4.95965800	-1.53885000	0.91320700
H	5.38111000	-2.52879300	1.14083600
H	4.46915800	-1.15807700	1.81758800
C	2.61102500	-1.47938600	0.05793700
H	2.15313200	-1.21578900	1.00995500
C	4.14552500	-2.00382100	-1.43007300
H	5.13965800	-2.22189100	-1.80904900
C	2.90925300	-1.97955000	-2.01933800
H	2.64276700	-2.17917500	-3.05442400
C	-1.81538300	0.06003200	-1.69305900
C	-1.90121400	1.44243200	-1.68544800
C	-3.10585600	2.13654100	-1.63390100
C	-4.29395200	1.41115100	-1.58333100
C	-4.25335200	0.01847700	-1.59760100
C	-3.02003100	-0.62603000	-1.65425500

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Optimized coordinates of **4** from PBE0-D3(BJ)/def2-SVP in G16

Ag	-0.43713600	-1.03866100	-1.02995200
F	-3.10549300	-0.33747200	-2.56049900
F	-5.68164000	-0.35453300	-1.80963200
F	-6.40449800	-1.42245400	0.57872400

F	-4.51381000	-2.46217900	2.23041600
F	-1.93044300	-2.42193100	1.52382400
N	1.60834100	-0.57596600	-1.47261000
N	3.52537700	0.53163200	-1.65494300
C	2.18638400	0.60154700	-1.41628200
H	1.66327700	1.53732900	-1.21101700
C	2.60121100	-1.48714800	-1.77918900
C	2.53662600	-2.86937500	-1.96608600
H	1.58632900	-3.39646700	-1.86212100
C	3.71728800	-3.52806900	-2.28034000
H	3.70366000	-4.60865000	-2.43598300
C	4.93499400	-2.83432400	-2.40305400
H	5.84075300	-3.38846300	-2.65858100
C	5.01409400	-1.45785300	-2.21824100
H	5.96314500	-0.93015100	-2.33403700
C	3.82433900	-0.79822600	-1.90420900
C	-2.41572700	-1.41667000	-0.57063800
C	-3.41496200	-0.90084400	-1.38308800
C	-4.76013400	-0.89611700	-1.02293000
C	-5.13335700	-1.42701300	0.20996900
C	-4.16208000	-1.96429800	1.05161700
C	-2.83178300	-1.93858600	0.64291800
C	4.44819700	1.64421700	-1.72580900
H	4.13464700	2.34835300	-2.50884500
H	5.42243900	1.23603500	-2.03352900
C	4.61616100	2.46497100	-0.46247500
N	4.48242500	3.77488600	-0.66089500
C	4.67516200	4.61634300	0.34860200
H	4.54209800	5.68087700	0.12790100
C	5.02847200	4.19348700	1.62746700
H	5.18633100	4.91389300	2.43196200
C	5.16800500	2.82762700	1.84195400
H	5.43982200	2.44815200	2.83125700
C	4.95594200	1.92690400	0.79497100
Ag	-0.35619100	0.65191100	1.56101700
F	-0.60823200	2.34834200	-1.07423900
F	-2.73461800	3.17874100	-2.49131000
F	-5.24830400	2.84606200	-1.50872000
F	-5.61889300	1.68872300	0.91284200
F	-3.50824100	0.87559700	2.36600500
N	1.58519300	-0.17239400	1.97732900
N	3.74484700	-0.09491300	1.44770700
C	5.03905100	0.45088000	1.07386700
H	5.39256800	-0.10968700	0.19553100

H	5.76069700	0.26646100	1.88625400
C	2.62627400	0.60248000	1.77410200
H	2.61229800	1.68896500	1.83310700
C	2.02655900	-1.46884700	1.78016700
C	1.33137600	-2.68119700	1.81670400
H	0.26110700	-2.70634800	2.02591100
C	2.05695300	-3.83430900	1.54952800
H	1.54727800	-4.79983900	1.56749300
C	3.43259300	-3.79176300	1.25105300
H	3.96139600	-4.72468500	1.04489800
C	4.13255300	-2.59344000	1.19575000
H	5.19294300	-2.56631900	0.94086200
C	3.39951500	-1.43585100	1.45733400
C	-1.97795100	1.61276500	0.72104900
C	-1.83830200	2.20452900	-0.52284900
C	-2.91293500	2.63586500	-1.29317700
C	-4.20248400	2.46075700	-0.79538600
C	-4.38721200	1.87933900	0.45773900
C	-3.27484700	1.46805100	1.18830300

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Optimized coordinates of **1a** from PBE0-D3(BJ)/def2-SVP in G16

Ag	0.77200400	-0.21889800	-1.47582700
Ag	0.76762600	-0.09865500	1.59348100
F	-2.19355200	-1.03039200	-2.24947500
F	-4.55924500	0.11449100	-1.70720800
F	-4.66150500	2.59732200	-0.61901200
F	-2.35995700	3.93690700	-0.06895000
F	0.01589300	2.81655700	-0.58897300
F	-0.32352800	-2.99054400	0.58256800
F	-2.80189200	-3.80619100	-0.03137100
F	-4.93555100	-2.19456600	0.45404300
F	-4.56566200	0.24837200	1.57274800
F	-2.09682900	1.08175500	2.22043900
N	2.60372800	-1.29660500	-1.21141000
N	4.74378300	-1.72002100	-0.94907700
N	2.66690600	0.88365600	1.42499600
N	4.08183800	2.35121300	0.60760700
C	3.82614800	-0.91272100	-1.52251000
H	4.08879700	-0.06739700	-2.15603600
C	4.05954800	-2.66741500	-0.22519500
H	4.56986800	-3.44772000	0.33329100
C	2.72764100	-2.39304600	-0.39637900
H	1.85514400	-2.89882700	0.01254600

C	-0.99231600	0.85356800	-1.47275300
C	-2.19175400	0.20982300	-1.74217800
C	-3.43441400	0.77737800	-1.47242400
C	-3.49181900	2.04517700	-0.89686200
C	-2.31103000	2.73064200	-0.62168900
C	-1.09782200	2.11484900	-0.91339400
C	6.17680800	-1.58289700	-1.03670400
H	6.42204700	-0.82543100	-1.79148800
H	6.63554300	-2.53516600	-1.33689600
H	6.59724600	-1.26880900	-0.06972100
H	5.31547800	3.24689800	-0.83683900
C	4.58138800	3.52643200	-0.06782000
H	5.05390200	4.21472400	0.64760300
H	3.74331900	4.04210200	-0.55245500
C	2.78541300	1.99455000	0.72025400
H	1.95983000	2.54476900	0.26773200
C	4.82919000	1.41192900	1.27930500
H	5.91100100	1.48364500	1.35823000
C	3.93226600	0.50356300	1.78178100
H	4.11946700	-0.38871100	2.37451900
C	-1.11409200	-0.93627600	1.47043600
C	-1.35177500	-2.16869400	0.88553500
C	-2.62205600	-2.62308500	0.54264000
C	-3.71732400	-1.79724000	0.78384800
C	-3.52404300	-0.55041700	1.37533400
C	-2.23189200	-0.14714900	1.70072100

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Optimized coordinates of **2a** from PBE0-D3(BJ)/def2-SVP in G16

Ag	0.07429400	0.06746800	-1.44483700
Ag	-0.39103700	-0.42383400	1.62862200
F	2.93880500	-0.87729900	-2.33393800
F	5.40600400	0.03733200	-1.80742100
F	5.73985300	2.36331100	-0.44604900
F	3.57496800	3.77818700	0.38022500
F	1.09881400	2.89524300	-0.14668800
F	0.92219200	-3.11612200	0.33581500
F	3.46554000	-3.71171600	-0.25684900
F	5.47661500	-2.03410600	0.48340800
F	4.91732100	0.24161200	1.83720300
F	2.37289900	0.87266300	2.43560900
N	-1.76379100	-1.03383800	-1.42410500
N	-3.12608600	-2.65248900	-0.74738900
N	-2.40928600	0.28233500	1.65123600

N	-4.62692200	0.37588900	1.77109100
C	-1.84423600	-2.23663700	-0.89822000
H	-0.98656000	-2.83469900	-0.58573200
C	-3.06182100	-0.61631100	-1.63837200
C	-3.56207500	0.57432000	-2.17170300
H	-2.88388900	1.36636000	-2.49314600
C	-4.94084600	0.70667900	-2.25865000
H	-5.36415300	1.62694800	-2.66527200
C	-5.80905700	-0.31663000	-1.83160900
H	-6.88780400	-0.17454900	-1.93050600
C	-5.32681500	-1.50868700	-1.30055800
H	-6.00233400	-2.30612000	-0.98433700
C	-3.93954300	-1.63551400	-1.21108400
C	1.91683600	0.98653600	-1.29324500
C	3.05183500	0.29489400	-1.69010900
C	4.34551900	0.74028400	-1.42946200
C	4.52084200	1.92561800	-0.71912100
C	3.40758300	2.65057700	-0.29980000
C	2.13744000	2.16211500	-0.59513400
C	-3.50240000	-0.32439100	2.05640200
H	-3.53117200	-1.28181300	2.57620700
C	-2.82396200	1.45964700	1.05267800
C	-2.08700000	2.47472400	0.43515300
H	-0.99781800	2.42915600	0.37041500
C	-2.80150200	3.54055100	-0.09506900
H	-2.25712700	4.35144800	-0.58344200
C	-4.20656400	3.60620800	-0.01231400
H	-4.72444300	4.46800600	-0.43914900
C	-4.94923300	2.60434400	0.59953700
H	-6.03779600	2.65461100	0.65639000
C	-4.22921100	1.53059500	1.12483800
C	1.54722000	-1.10621100	1.43905700
C	1.88590900	-2.25806900	0.75060200
C	3.19295200	-2.60308100	0.41922100
C	4.22378100	-1.74457900	0.79232000
C	3.93118400	-0.57915300	1.49878700
C	2.60518400	-0.28223900	1.79892700
C	-5.98427700	-0.00670700	2.05986500
H	-6.47002500	0.74517200	2.69945400
H	-6.55552800	-0.11190500	1.12568500
H	-5.98600200	-0.96895300	2.58708700
C	-3.55835100	-3.92094000	-0.22002500
H	-4.20955000	-3.77463900	0.65514800
H	-4.11029700	-4.49265800	-0.98107400

H	-2.67944500	-4.50002400	0.08919900
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Optimized coordinates of **1b** from PBE0-D3(BJ)/def2-SVP in G16

Ag	0.58075700	1.55520500	-0.16561600
Ag	-0.58078400	-1.55502000	0.16438800
F	-1.84216000	1.56172000	-2.34396200
F	-4.51351100	1.39255700	-2.05178400
F	-5.60854600	1.25686500	0.41947800
F	-4.02436700	1.26590100	2.61946700
F	-1.35091700	1.41135300	2.35650200
F	1.84029100	-1.56017300	2.34398700
F	4.51189800	-1.39121400	2.05385600
F	5.60891100	-1.25726800	-0.41668600
F	4.02649900	-1.26753400	-2.61786300
F	1.35281900	-1.41270700	-2.35694300
N	2.71420300	1.75838300	-0.22100400
N	4.79889300	1.66670800	0.47114200
N	-2.71432300	-1.75843700	0.21961600
N	-4.79932700	-1.66659300	-0.47152400
C	3.50035000	1.61503600	0.83014300
H	3.17203300	1.45282700	1.85541000
C	4.84150800	1.84467100	-0.89032400
H	5.77855300	1.89307000	-1.43766700
C	3.53799900	1.90256600	-1.30745000
H	3.14807900	2.02812700	-2.31452300
C	-1.48740900	1.54145600	-0.00186700
C	-2.33564400	1.53804900	-1.09856300
C	-3.72156000	1.46471200	-0.97962300
C	-4.28905600	1.38478800	0.28863400
C	-3.47521600	1.38846400	1.41659600
C	-2.09497200	1.46191300	1.24314500
C	5.93266200	1.45786100	1.34297300
H	5.58209400	1.41711900	2.38098800
H	6.64973900	2.28382300	1.23960500
H	6.42219100	0.50511800	1.10120200
H	-6.42237600	-0.50423300	-1.10084500
C	-5.93355000	-1.45733800	-1.34264800
H	-6.65103800	-2.28284500	-1.23849200
H	-5.58371200	-1.41716500	-2.38093300
C	-3.50095000	-1.61459900	-0.83108600
H	-3.17311000	-1.45196700	-1.85643800
C	-4.84131000	-1.84528300	0.88987300
H	-5.77811500	-1.89398200	1.43759900

C	-3.53760700	-1.90326900	1.30637200
H	-3.14719300	-2.02918800	2.31321000
C	1.48745700	-1.54145000	0.00159100
C	2.33479300	-1.53735200	1.09898300
C	3.72080300	-1.46411100	0.98110200
C	4.28931300	-1.38501600	-0.28675500
C	3.47636700	-1.38935000	-1.41536100
C	2.09598100	-1.46263800	-1.24297800

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Optimized coordinates of **2b** from PBE0-D3(BJ)/def2-SVP in G16

Ag	0.23052200	1.54038300	-0.58727500
Ag	-0.23063400	-1.54046600	0.58744500
F	-2.33230500	3.05072700	0.73389500
F	-4.97507600	2.75060400	0.36493200
F	-5.90517100	0.86078700	-1.35657700
F	-4.16886300	-0.68712300	-2.74554500
F	-1.52292000	-0.38927800	-2.40945600
F	2.33169200	-3.05035900	-0.73471500
F	4.97463800	-2.75060500	-0.36628600
F	5.90529600	-0.86151500	1.35571100
F	4.16944500	0.68617900	2.74549200
F	1.52341700	0.38874700	2.40989600
N	2.35284400	1.75789500	-0.55531400
N	4.44877500	2.18262500	0.04460400
N	-2.35287800	-1.75765400	0.55571000
N	-4.44890700	-2.18248600	-0.04380700
C	3.13580500	2.45035700	0.24203600
H	2.79400600	3.15259400	1.00144000
C	3.18851100	0.97094700	-1.32598800
C	2.89393900	0.01011200	-2.29743400
H	1.85851200	-0.21100900	-2.56539000
C	3.96202900	-0.66572100	-2.86891700
H	3.76872200	-1.43828500	-3.61542600
C	5.29213800	-0.39614000	-2.49138300
H	6.10070300	-0.96426800	-2.95548200
C	5.60036900	0.55721600	-1.52996300
H	6.63011200	0.74499500	-1.22304900
C	4.52169700	1.23119600	-0.95486800
C	-1.81390100	1.37080400	-0.84800400
C	-2.73926400	2.14493000	-0.16332200
C	-4.11729200	2.01362800	-0.33069100
C	-4.59626200	1.05713300	-1.22038900
C	-3.70118600	0.26460900	-1.93245400

C	-2.33593300	0.43898200	-1.73100800
C	5.56216900	2.68873500	0.80746400
H	6.27984200	3.19960200	0.14894400
H	6.06414700	1.86172600	1.32913200
C	-5.56244400	-2.68876500	-0.80631500
H	-6.06477300	-1.86190300	-1.32786300
H	-6.27984300	-3.19980900	-0.14762500
C	-3.13596900	-2.45033200	-0.24131300
H	-2.79428700	-3.15294600	-1.00042400
C	-3.18842600	-0.97045800	1.32626500
C	-2.89368800	-0.00937800	2.29740900
H	-1.85822600	0.21174200	2.56521000
C	-3.96166800	0.66666300	2.86883900
H	-3.76821400	1.43941000	3.61512300
C	-5.29183700	0.39706900	2.49151900
H	-6.10031700	0.96537600	2.95554400
C	-5.60022300	-0.55655100	1.53041300
H	-6.63001500	-0.74442600	1.22372200
C	-4.52166300	-1.23074100	0.95538400
C	1.81386800	-1.37085100	0.84781400
C	2.73898800	-2.14487900	0.16267300
C	4.11706100	-2.01376400	0.32974300
C	4.59634500	-1.05767600	1.21973600
C	3.70150000	-0.26526300	1.93219700
C	2.33617400	-0.43938000	1.73100300
H	5.19320300	3.40127200	1.55481500
H	-5.19355100	-3.40120200	-1.55380200