Supporting Material

Structural Characterization and Gas-phase Studies of the $[Ag_{10}H_8L_6]^{2+}$ Nanocluster Dication

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S.1. Spectroscopic Characterization

S.1.1. NMR Spectra

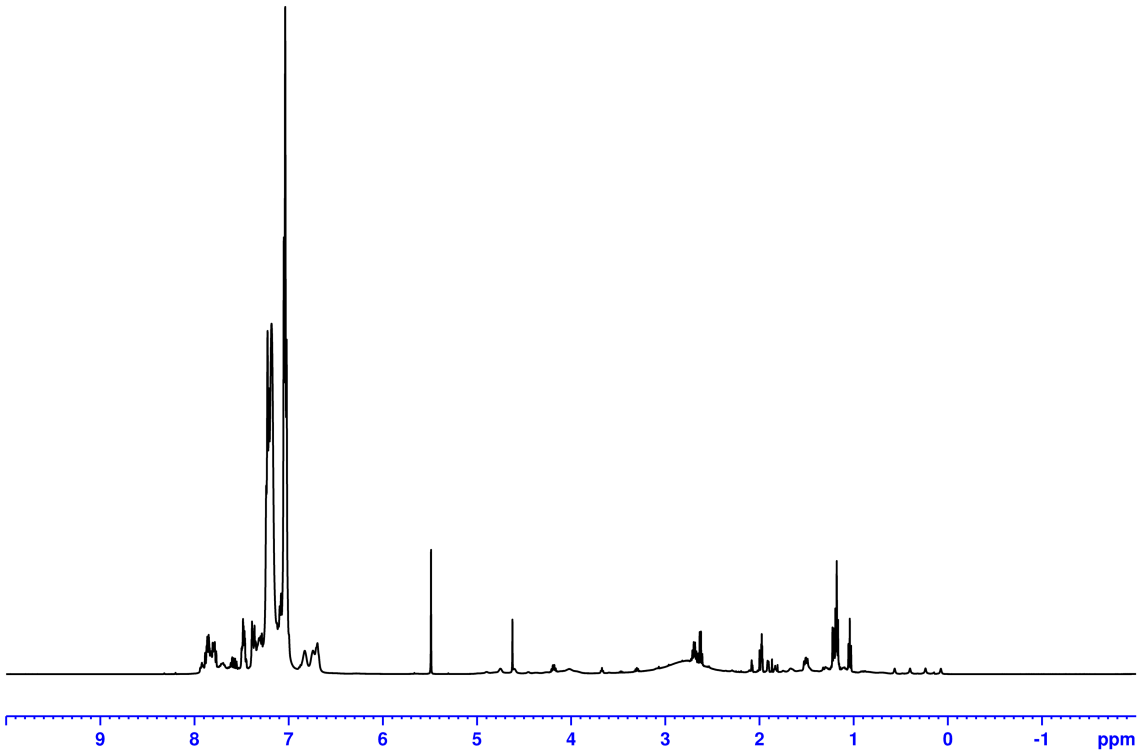

Figure S1: ^{1}H NMR spectrum of crude product containing **7(BF$_4$)$_2$** in CD_3CN.

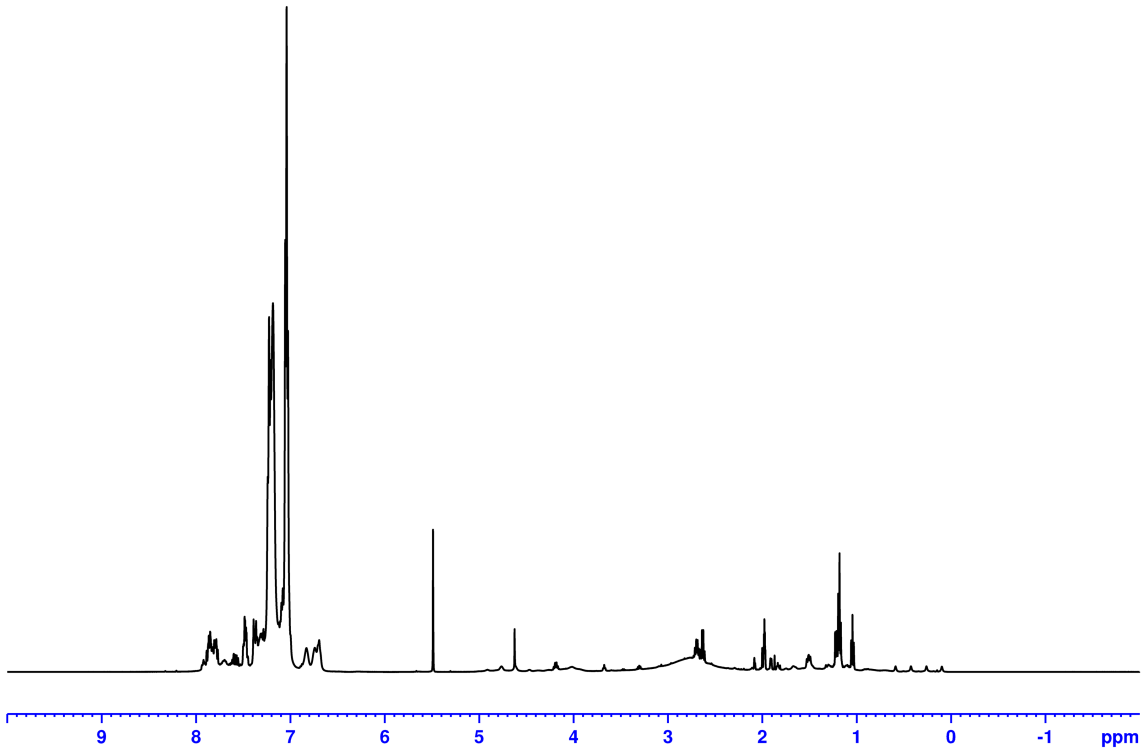

Figure S2: $^{1}H\{^{31}P\}$ NMR spectrum of crude product containing **7(BF$_4$)$_2$** in CD_3CN.

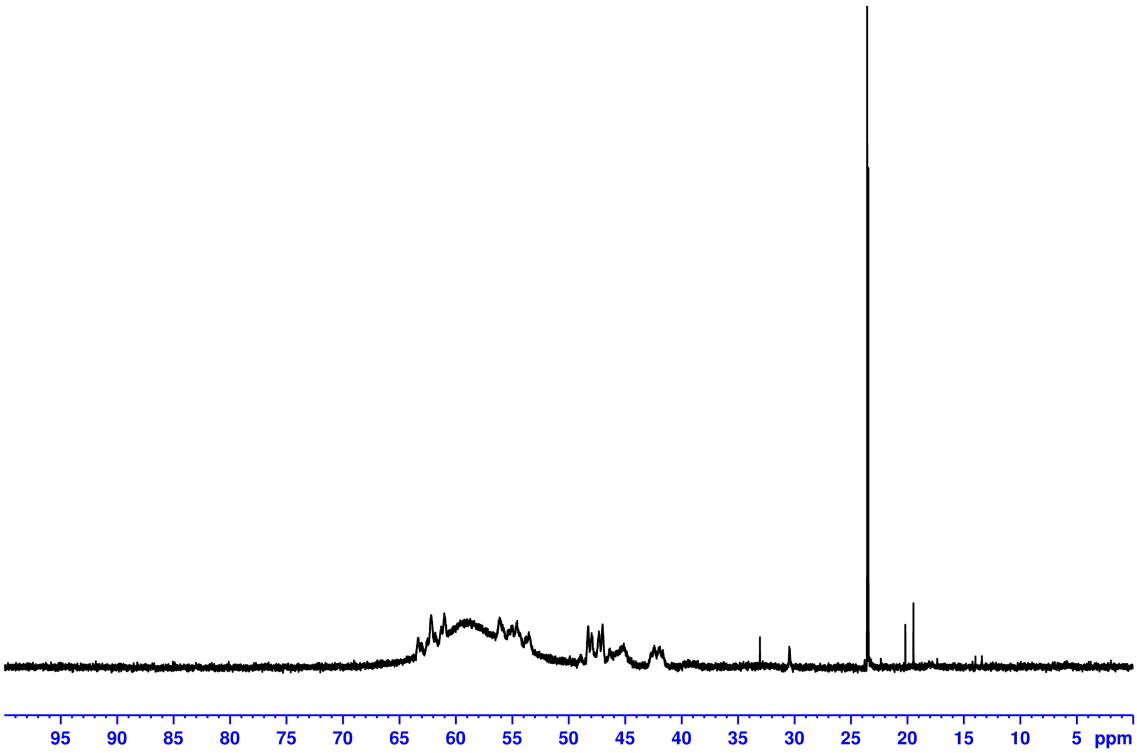

Figure S3: $^{31}P\{^{1}H\}$ NMR spectrum of crude product containing **7(BF$_4$)$_2$** in CD_3CN.

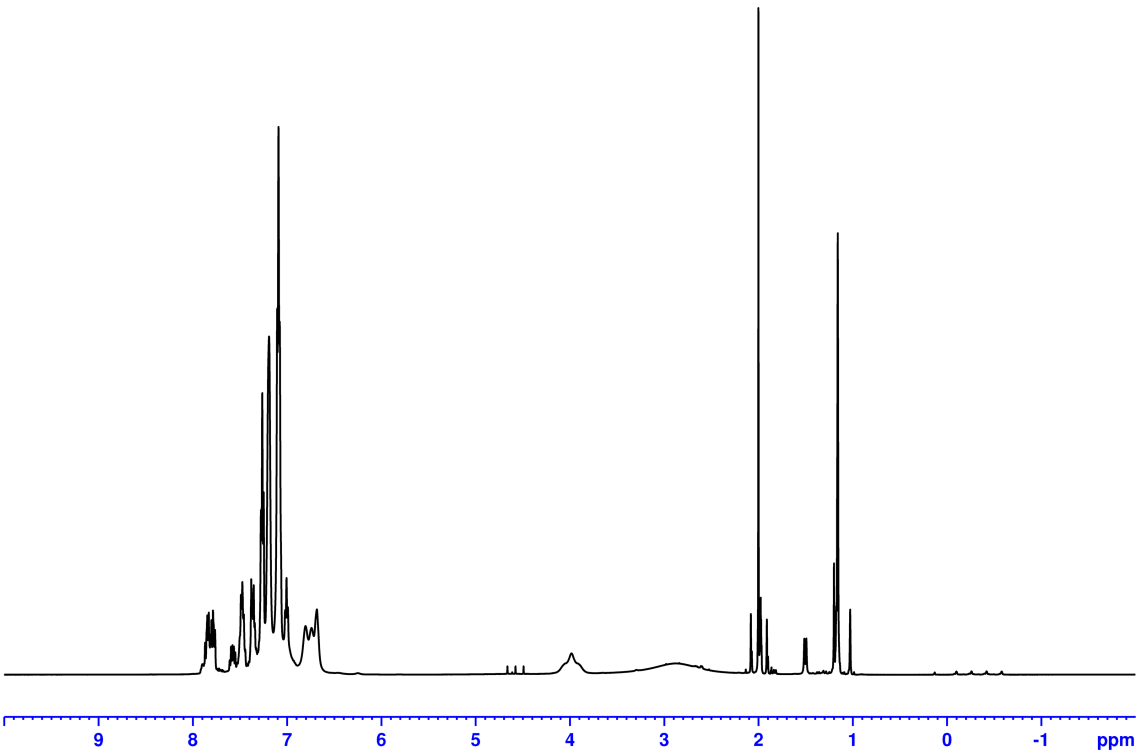

Figure S4: ^{1}H NMR spectrum of crude product containing **7$_D$(BF$_4$)$_2$** in CD_3CN.

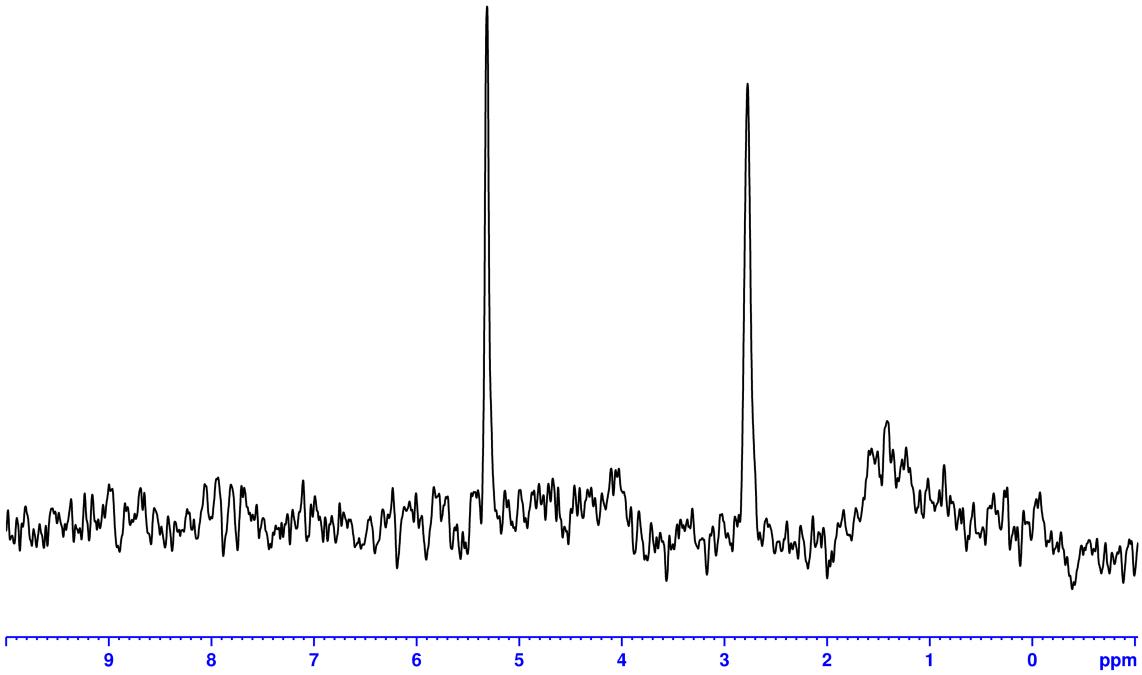

Figure S5: ^{2}H NMR spectrum of crude product containing $\mathbf{7_D(BF_4)_2}$ in CH_2Cl_2.

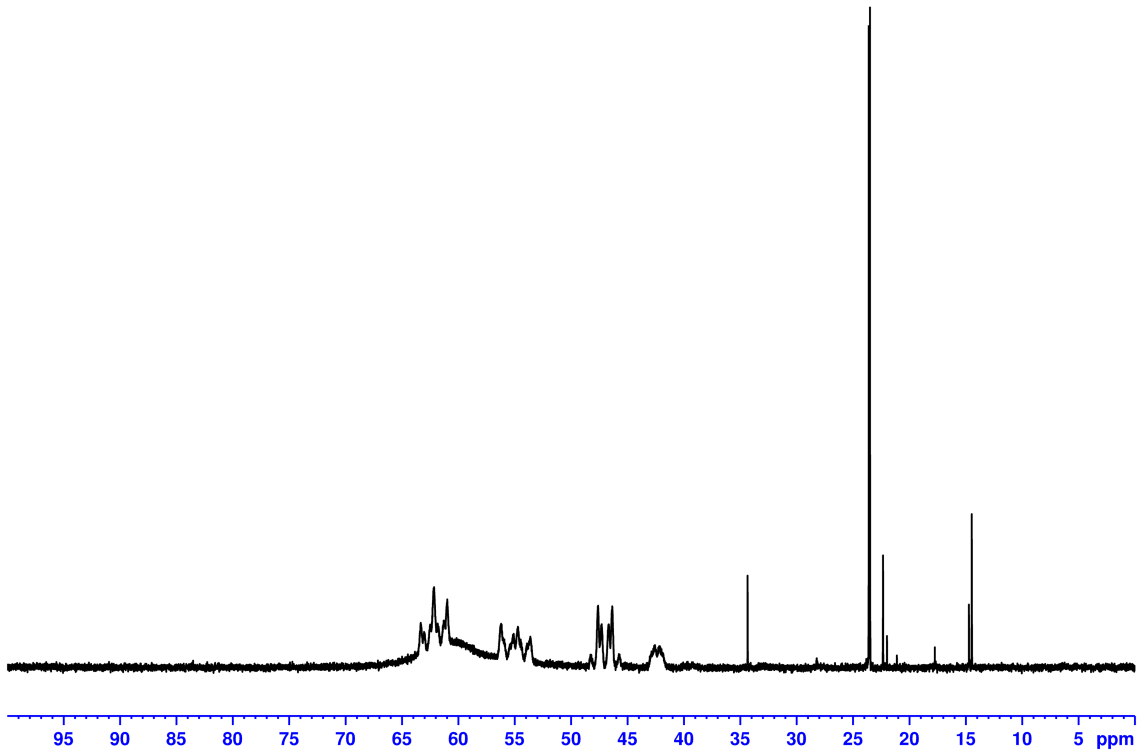

Figure S6: $^{31}P\{^{1}H\}$ NMR spectrum of crude product containing $\mathbf{7_D(BF_4)_2}$ in CD_3CN.

S.1.2. IR Spectra

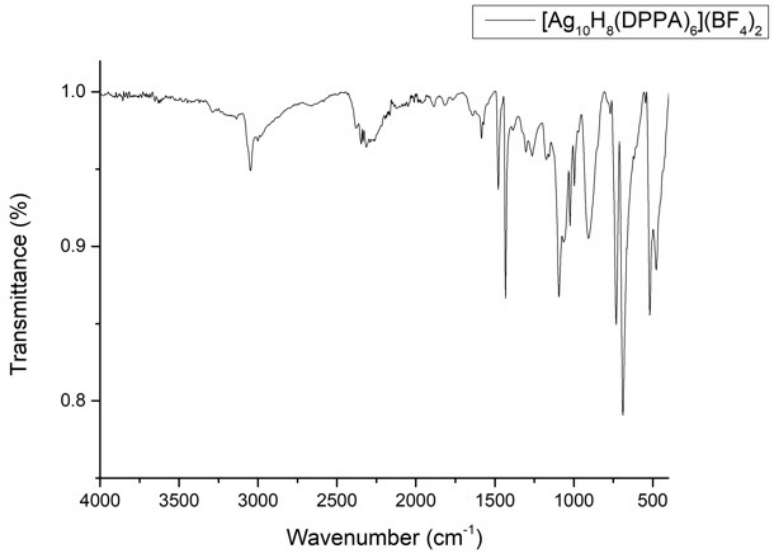

Figure S7: ATR-FTIR spectrum of crude product containing **7(BF$_4$)$_2$**. Spectrum was collected from a sample mixture of silver clusters including **7(BF$_4$)$_2$** with an average of 32 scans.

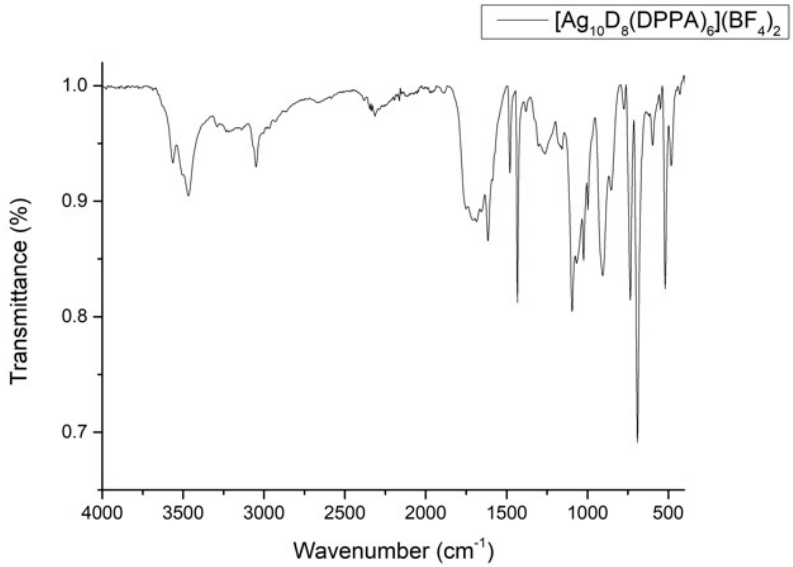

Figure S8: ATR-FTIR spectrum of crude product containing **7$_D$(BF$_4$)$_2$**. Spectrum was collected from a sample mixture of silver clusters including **7$_D$(BF$_4$)$_2$** with an average of 32 scans.

S.1.3. UV-Vis Spectra

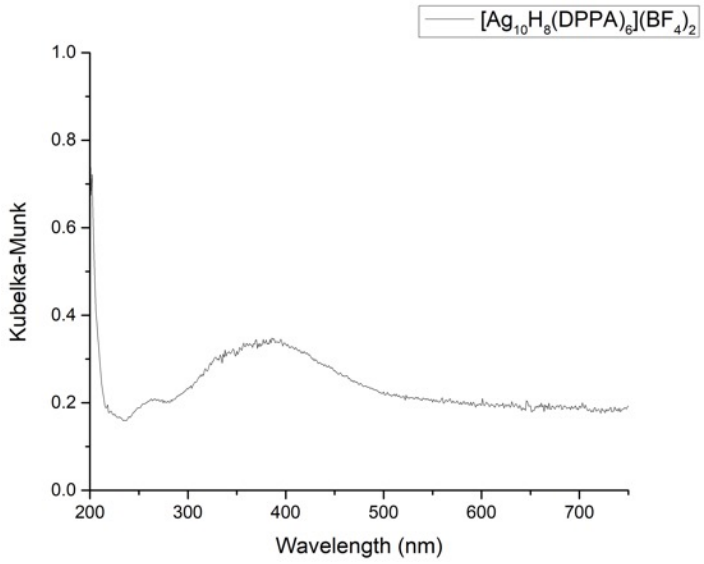

Figure S9: Diffuse reflectance spectra of crude product containing **7(BF$_4$)$_2$**.

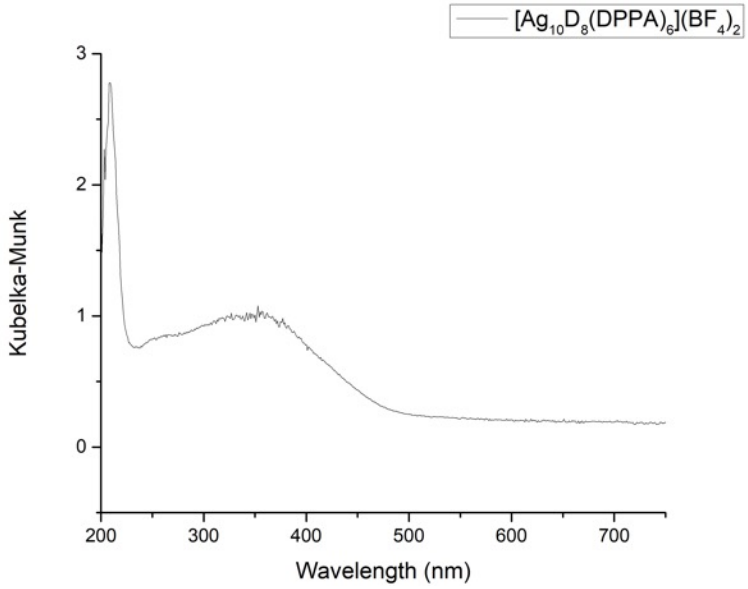

Figure S10: Diffuse reflectance spectra of crude product containing **7$_D$(BF$_4$)$_2$**.

S.2. X-ray Crystallographic Data

S.2.1. $[Ag_{10}H_8(dppa)_6](BF_4)_2$, $7(BF_4)_2$

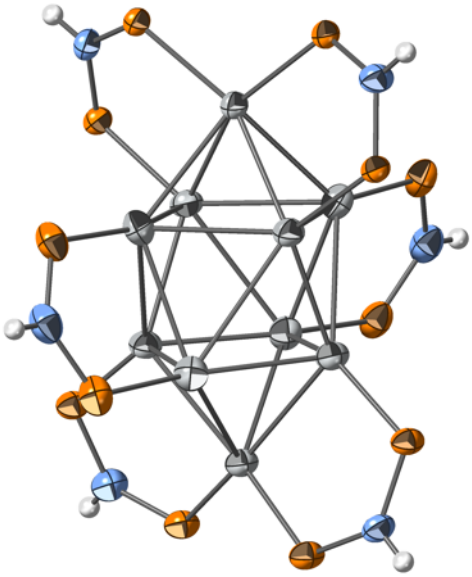

Figure S11: Solid-state structure of the cationic portion of **$7(BF_4)_2$** (50% displacement ellipsoids). All phenyl groups omitted for clarity. Color legend: Ag (silver); P (orange); N (blue) and H (white).

Additional details for $7(BF_4)_2$: This compound crystallized in the orthorhombic space group Pbcn with half a molecule within the asymmetric unit. The data for this compound are of poor quality, the R(int) and final R_1 are elevated, presumably due to solvent loss during the crystal selection stage. The data present herein are sufficient for discussion of molecular connectivity, but are not appropriate for detailed discussion of structural metrics. Numerous level A and B checkcif alerts emanate from sizeable peaks and holes of electron density proximal to the atoms of the Ag_{10} core.

Table S1: Crystal data and structure refinement for **7(BF$_4$)$_2$**.

CCDC number	1919380
Empirical formula	$C_{148}H_{134}Ag_{10}B_2Cl_8F_8N_6P_{12}$
Formula weight	3904.16
Temperature/K	100.01(10)
Crystal system	orthorhombic
Space group	Pbcn
a/Å	28.1498(7)
b/Å	17.1737(3)
c/Å	30.4308(7)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	14711.4(6)
Z	4
ρ_{calc}g/cm^3	1.763
μ/mm^{-1}	13.513
F(000)	7728.0
Crystal size/mm^3	0.376 × 0.267 × 0.195
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	5.808 to 156.596
Index ranges	$-35 \leq h \leq 35$, $-21 \leq k \leq 13$, $-35 \leq l \leq 38$
Reflections collected	73646
Independent reflections	15461 [R_{int} = 0.2045, R_{sigma} = 0.1209]
Data/restraints/parameters	15461/1001/874
Goodness-of-fit on F^2	1.063
Final R indexes [I>=2σ (I)]	R_1 = 0.1210, wR_2 = 0.3062
Final R indexes [all data]	R_1 = 0.1637, wR_2 = 0.3495
Largest diff. peak/hole / e Å^{-3}	2.73/-3.62

Table S2: Key bond distances of X-ray crystallography for **7(BF$_4$)$_2$**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ag1	Ag4	2.8679(14)	Cl4	C74	1.75(3)	C57	C58	1.35(2)
Ag1	Ag2	2.8714(14)	Cl3	C74	1.71(2)	C21	C22	1.41(3)
Ag1	Ag3	2.9783(14)	C67	C68	1.32(3)	C52	C51	1.40(4)
Ag1	Ag5	3.0037(14)	C67	C72	1.35(2)	C50	C51	1.39(3)
Ag1	P4	2.499(3)	C11	C12	1.42(2)	F2	B1	1.36(2)
Ag1	P5	2.505(3)	C11	C10	1.31(3)	F1	B1	1.39(3)
Ag4	Ag4^1	2.751(2)	C31	C36	1.40(2)	F3	B1	1.35(3)
Ag4	Ag3	2.8642(14)	C31	C32	1.36(2)	C42	C37	1.41(2)
Ag4	Ag5	2.8929(15)	C37	C38	1.37(2)	C42	C41	1.39(2)
Ag4	Ag5^1	3.2109(15)	C2	C3	1.41(2)	C56	C57	1.38(2)
Ag4	P6	2.473(3)	C28	C27	1.37(3)	C56	C55	1.38(2)
Ag2	Ag2^1	2.782(2)	C28	C29	1.34(3)	C61	C62	1.35(2)
Ag2	Ag3	2.8639(15)	C41	C40	1.34(3)	C61	C66	1.35(3)
Ag2	Ag3^1	3.1230(15)	C13	C18	1.38(2)	F4	B1	1.36(3)
Ag2	Ag5	2.8747(15)	C13	C14	1.36(3)	C25	C30	1.39(2)
Ag2	P3	2.467(3)	C48	C47	1.36(3)	C25	C26	1.37(2)
Ag3	Ag5^1	2.9287(16)	C10	C9	1.39(3)	C43	C48	1.41(3)
Ag3	P2	2.472(4)	C35	C36	1.36(2)	C43	C44	1.40(3)
Ag5	P1^1	2.502(4)	C35	C34	1.37(3)	C1	C2	1.36(2)
P3	N2	1.721(13)	C49	C54	1.36(3)	C1	C6	1.42(2)
P3	C25	1.812(15)	C49	C50	1.40(3)	C7	C12	1.38(2)
P3	C31	1.841(15)	C6	C5	1.42(2)	C7	C8	1.38(3)
P6	N3	1.721(13)	C54	C53	1.38(3)	C59	C58	1.39(3)
P6	C61	1.808(15)	C20	C19	1.38(2)	C38	C39	1.43(3)
P6	C67	1.845(16)	C20	C21	1.39(3)	C8	C9	1.41(3)
P4	N2	1.685(12)	C60	C59	1.38(3)	C14	C15	1.45(3)
P4	C43	1.841(16)	C60	C55	1.38(2)	C39	C40	1.36(3)
P4	C37	1.827(16)	C53	C52	1.43(4)	C45	C46	1.35(3)
P5	N3	1.691(12)	C17	C18	1.40(2)	C30	C29	1.41(3)
P5	C49	1.853(17)	C17	C16	1.37(3)	C68	C69	1.41(3)

P5	C55	1.836(17)	C5	C4	1.39(3)	C15	C16	1.37(3)
P1	N1	1.684(15)	C47	C46	1.33(4)	C22	C23	1.31(3)
P1	C1	1.839(17)	C34	C33	1.37(3)	C26	C27	1.34(3)
P1	C7	1.849(17)	C32	C33	1.40(3)	C24	C23	1.37(3)
P2	N1	1.705(15)	C44	C45	1.34(3)	C70	C71	1.31(3)
P2	C13	1.830(16)	C4	C3	1.40(2)	C70	C69	1.41(3)
P2	C19	1.816(18)	C64	C63	1.26(3)	C71	C72	1.38(3)
Cl1	C73	1.72(3)	C64	C65	1.33(3)	C62	C63	1.43(3)
Cl2	C73	1.79(2)	C19	C24	1.41(3)	C65	C66	1.35(3)

[1]1-X,+Y,1/2-Z

S.2.2. $[Ag_{10}H_8(dppa)_6](NO_3)_2$, $7(NO_3)_2$

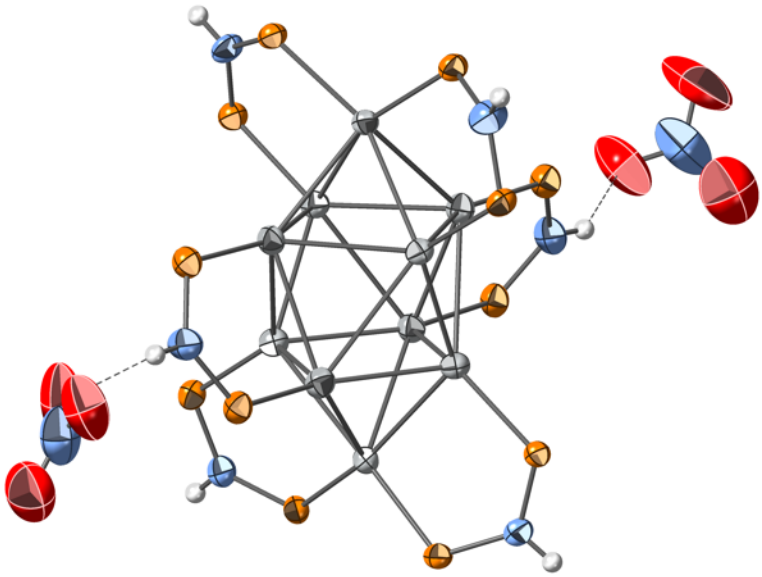

Figure S12: Solid-state structure of the cationic portion of $\mathbf{7(NO_3)_2}$ (50% displacement ellipsoids). All phenyl groups omitted for clarity. Color legend: Ag (silver); P (orange); N (blue); C (black) and H (white).

Additional details for $7(NO_3)_2$: Both nitrate groups and a single phenyl group were modelled as disordered over two sites. The lattice contained numerous solvent molecules that were best modelled as substitutionally disordered acetonitrile and water molecules. Most level B checkcif alerts emanate from close proximities of some of the disordered components.

Table S3: Crystal data and structure refinement for **7(NO$_3$)$_2$**.

CCDC number	1919381
Empirical formula	$C_{154}H_{142}Ag_{10}N_{11}O_{9.5}P_{12}$
Formula weight	3749.12
Temperature/K	100.00(10)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	16.53950(10)
b/Å	24.44690(10)
c/Å	38.1398(2)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	15421.43(14)
Z	4
ρ_{calc}g/cm^3	1.615
μ/mm^{-1}	11.602
F(000)	7476.0
Crystal size/mm^3	0.14 × 0.14 × 0.04
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.452 to 156.908
Index ranges	$-20 \leq h \leq 20$, $-30 \leq k \leq 28$, $-45 \leq l \leq 48$
Reflections collected	133405
Independent reflections	32323 [R_{int} = 0.0695, R_{sigma} = 0.0465]
Data/restraints/parameters	32323/577/1940
Goodness-of-fit on F^2	1.036
Final R indexes [I>=2σ (I)]	R_1 = 0.0486, wR_2 = 0.1330
Final R indexes [all data]	R_1 = 0.0527, wR_2 = 0.1369
Largest diff. peak/hole / e Å^{-3}	2.20/-1.47
Flack parameter	-0.017(3)

Table S4: Key bond distances of X-ray crystallography for **7(NO$_3$)$_2$**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ag1	Ag4	2.8647(8)	C103	C104	1.361(17)	C1F	C1G	1.36(3)
Ag1	Ag3	3.0001(8)	C103	C108	1.380(15)	C73	C78	1.351(17)
Ag1	Ag2	2.8961(9)	C13	C14	1.402(15)	C110	C111	1.382(15)
Ag1	Ag5	3.0307(9)	C133	C134	1.389(18)	C104	C105	1.425(18)
Ag1	P3	2.522(2)	C133	C138	1.403(15)	C63	C62	1.364(18)
Ag1	P1	2.541(2)	C121	C126	1.394(16)	C63	C64	1.420(19)
Ag10	Ag6	2.9654(9)	C121	C122	1.394(17)	C96	C95	1.389(18)
Ag10	Ag9	2.8653(8)	C91	C92	1.361(16)	C122	C123	1.379(19)
Ag10	Ag7	2.8854(9)	C91	C96	1.408(17)	C123	C124	1.38(2)
Ag10	Ag8	3.0278(9)	C79	C80	1.416(17)	C144	C143	1.402(16)
Ag10	P10	2.519(2)	C79	C84	1.370(17)	C124	C125	1.39(2)
Ag10	P12	2.519(2)	C115	C116	1.378(15)	C44	C45	1.377(17)
Ag4	Ag9	2.7705(9)	C115	C120	1.361(15)	C67	C68	1.404(17)
Ag4	Ag3	2.8826(9)	C61	C62	1.416(17)	C67	C72	1.38(2)
Ag4	Ag8	3.2372(9)	C61	C66	1.385(16)	C135	C136	1.33(2)
Ag4	Ag5	2.8612(9)	C19	C24	1.35(2)	C136	C137	1.39(3)
Ag4	P2	2.471(2)	C19	C20	1.377(19)	C80	C81	1.42(2)
Ag6	Ag9	2.9133(9)	C92	C93	1.39(2)	C74	C75	1.386(19)
Ag6	Ag7	2.9249(9)	C139	C140	1.386(17)	C7	C12	1.366(16)
Ag6	Ag2	3.2606(10)	C139	C144	1.405(15)	C7	C8	1.381(17)
Ag6	Ag5	2.9213(10)	C37	C42	1.407(18)	C105	C106	1.39(2)
Ag6	P8	2.504(2)	C37	C38	1.389(17)	C100	C101	1.41(2)
Ag9	Ag8	2.8742(9)	C97	C98	1.364(17)	C100	C99	1.359(19)
Ag9	Ag5	3.2145(10)	C97	C102	1.394(15)	C84	C83	1.37(2)
Ag9	P11	2.482(3)	C65	C64	1.39(2)	C111	C112	1.395(18)
Ag3	Ag7	3.2162(9)	C65	C66	1.378(19)	C112	C113	1.384(18)
Ag3	Ag2	2.9276(9)	C48	C47	1.403(19)	C98	C99	1.410(18)
Ag3	Ag8	2.9342(10)	C16	C17	1.361(19)	C86	C87	1.423(16)
Ag3	P5	2.510(2)	C16	C15	1.39(2)	C56	C57	1.39(2)
Ag7	Ag2	2.7879(9)	C85	C86	1.390(18)	C138	C137	1.37(2)

Ag7	Ag8	2.8585(9)	C85	C90	1.364(18)	C101	C102	1.413(19)
Ag7	P9	2.476(2)	C134	C135	1.379(18)	C114	C113	1.381(16)
Ag2	Ag5	2.8540(10)	C126	C125	1.369(16)	C87	C88	1.39(2)
Ag2	P4	2.476(3)	C140	C141	1.397(17)	C15	C14	1.394(17)
Ag8	P6	2.494(2)	C55	C56	1.401(19)	C90	C89	1.36(2)
Ag5	P7	2.490(2)	C55	C60	1.36(2)	C28	C27	1.39(3)
P3	C31	1.820(10)	C116	C117	1.405(15)	C28	C29	1.32(3)
P3	N2	1.676(8)	C25	C26	1.367(18)	C40	C41	1.32(2)
P3	C25	1.826(10)	C25	C30	1.33(2)	C40	C39	1.44(2)
P10	C109	1.846(11)	C49	C50	1.352(18)	C142	C141	1.379(19)
P10	N5	1.705(8)	C49	C54	1.366(19)	C142	C143	1.388(19)
P10	C115	1.842(10)	C73	C74	1.405(18)	C68	C69	1.369(19)
P5	N3	1.681(10)	C34	C33	1.43(3)	C22	C23	1.26(3)
P5	C55	1.832(11)	C26	C27	1.37(2)	C22	C21	1.40(3)
P5	C49	1.832(11)	C21	C20	1.34(2)	C83	C82	1.41(2)
P2	N1	1.681(8)	C29	C30	1.42(2)	C75	C76	1.40(2)
P2	C13	1.849(10)	N10	C151	1.162(13)	C57	C58	1.33(3)
P2	C19	1.842(11)	C151	C152	1.447(13)	C36	C35	1.412(18)
P9	N5	1.669(9)	O10	C145	1.63(3)	C35	C34	1.33(2)
P9	C103	1.839(10)	O10	C147	1.61(3)	C107	C108	1.391(17)
P9	C97	1.838(10)	C146	C145	1.59(4)	C107	C106	1.32(2)
P8	N4	1.683(9)	C147	C148	1.62(4)	C45	C46	1.35(2)
P8	C91	1.848(12)	N11	C153	1.152(13)	C117	C118	1.35(2)
P8	C85	1.829(12)	N11	C1H	1.120(12)	C59	C58	1.38(3)
P11	N6	1.680(10)	C153	C154	1.455(13)	C59	C60	1.37(2)
P11	C121	1.837(11)	N8	O6	1.256(13)	C76	C77	1.41(3)
P11	C127	1.850(15)	N8	O5	1.233(13)	C12	C11	1.393(17)
P11	C1F	1.87(2)	N8	O4	1.235(13)	C88	C89	1.36(3)
P1	N1	1.703(8)	N9	C149	1.150(12)	C50	C51	1.37(2)
P1	C1	1.808(11)	C149	C150	1.462(13)	C93	C94	1.35(2)
P1	C7	1.839(10)	N7A	O1A	1.246(13)	C41	C42	1.395(18)
P4	N2	1.699(9)	N7A	O3A	1.236(13)	C77	C78	1.38(2)

P4	C43	1.837(10)	N7A	O2A	1.245(13)	C69	C70	1.37(3)
P4	C37	1.807(11)	N7	O2	1.241(13)	C81	C82	1.32(2)
P12	N6	1.689(10)	N7	O3	1.240(12)	C51	C52	1.39(3)
P12	C133	1.822(11)	N7	O1	1.242(13)	C23	C24	1.44(2)
P12	C139	1.844(10)	C1A	C1H	1.455(13)	C39	C38	1.38(2)
P7	N4	1.691(9)	N12	C155	1.146(13)	C72	C71	1.41(2)
P7	C79	1.821(11)	C155	C156	1.455(13)	C95	C94	1.363(19)
P7	C73	1.829(12)	N8A	O4A	1.242(13)	C47	C46	1.37(2)
P6	N3	1.695(10)	N8A	O6A	1.249(13)	C118	C119	1.39(2)
P6	C61	1.819(11)	N8A	O5A	1.257(13)	C52	C53	1.35(3)
P6	C67	1.832(11)	C131	C132	1.383(16)	C11	C10	1.40(2)
C109	C110	1.382(14)	C131	C130	1.384(17)	C2	C3	1.37(2)
C109	C114	1.393(14)	C132	C127	1.386(17)	C6	C5	1.421(19)
C31	C36	1.388(16)	C127	C128	1.373(17)	C53	C54	1.397(18)
C31	C32	1.365(17)	C128	C129	1.390(16)	C5	C4	1.25(3)
C18	C13	1.364(15)	C129	C130	1.379(18)	C32	C33	1.39(2)
C18	C17	1.374(16)	C1B	C1C	1.35(3)	C9	C8	1.409(19)
C1	C2	1.398(18)	C1B	C1G	1.36(3)	C9	C10	1.41(2)
C1	C6	1.336(19)	C1C	C1D	1.36(3)	C120	C119	1.397(18)
C43	C48	1.348(17)	C1D	C1E	1.35(3)	C71	C70	1.35(3)
C43	C44	1.409(16)	C1E	C1F	1.36(3)	C4	C3	1.42(3)

S.2.3. $[Ag_2(\mu\text{-}P(Ph)_2NPPh_2)_2]$, 8

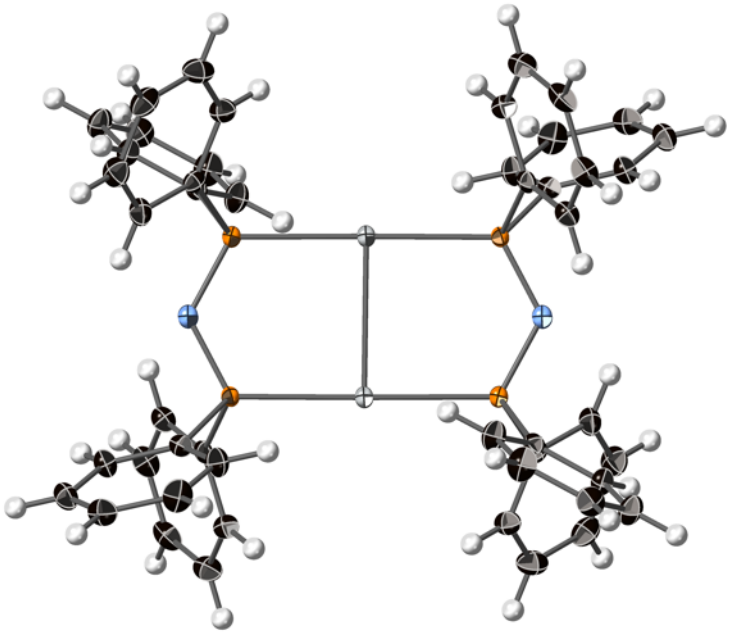

Figure S13: Solid-state structure of **8** (50% displacement ellipsoids). The complete dimer was generated for clarity using a [1]1-X,1-Y,-Z symmetry operation. All low occupancy phenyl groups omitted for clarity. Color legend: Ag (silver); P (orange); N (blue) and H (white).

Additional details for 8: This compound crystallized in the triclinic space group P-1 with a half dimer in the asymmetric unit. Two phenyl groups were modelled as disordered over two sites.

Table S5: Crystal data and structure refinement for **8**.

CCDC number	1919382
Empirical formula	$C_{24}H_{20}AgNP_2$
Formula weight	492.22
Temperature/K	100.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	8.8080(2)
b/Å	10.8055(2)
c/Å	11.8361(3)
α/°	77.075(2)
β/°	76.867(2)
γ/°	77.521(2)
Volume/Å^3	1052.91(4)
Z	2
ρcalcg/cm^3	1.553
μ/mm^{-1}	9.175
F(000)	496.0
Crystal size/mm3	0.15 × 0.14 × 0.04
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.802 to 154.002
Index ranges	$-10 \leq h \leq 11$, $-11 \leq k \leq 13$, $-14 \leq l \leq 14$
Reflections collected	13625
Independent reflections	4331 [R_{int} = 0.0440, R_{sigma} = 0.0401]
Data/restraints/parameters	4331/400/362
Goodness-of-fit on F^2	1.054
Final R indexes [I>=2σ (I)]	R_1 = 0.0323, wR_2 = 0.0857
Final R indexes [all data]	R_1 = 0.0329, wR_2 = 0.0863
Largest diff. peak/hole / e Å^{-3}	0.58/-1.36

Table S6: Key bond distances of X-ray crystallography for **8**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ag1	Ag1[1]	2.9070(3)	C4A	C3A	1.391(14)
Ag1	P1	2.4016(7)	C5A	C6A	1.401(7)
Ag1	P2[1]	2.4008(7)	C6A	C1A	1.392(14)
P1	N1	1.621(2)	C1A	C2A	1.388(14)
P1	C1A	1.841(19)	C2A	C3A	1.393(13)
P1	C1	1.817(16)	C4	C5	1.385(11)
P1	C7A	1.849(14)	C4	C3	1.387(13)
P1	C7	1.809(13)	C5	C6	1.380(7)
P2	N1	1.620(3)	C6	C1	1.399(12)
P2	C19	1.828(3)	C1	C2	1.394(12)
P2	C13	1.824(3)	C2	C3	1.398(11)
C20	C19	1.391(4)	C11A	C12A	1.400(10)
C20	C21	1.397(4)	C11A	C10A	1.384(10)
C19	C24	1.385(5)	C12A	C7A	1.394(11)
C13	C18	1.393(5)	C7A	C8A	1.387(10)
C13	C14	1.385(5)	C8A	C9A	1.395(10)
C18	C17	1.391(5)	C9A	C10A	1.372(10)
C21	C22	1.369(6)	C10	C9	1.369(9)
C24	C23	1.390(5)	C10	C11	1.392(9)
C14	C15	1.395(5)	C9	C8	1.404(10)
C16	C15	1.378(6)	C8	C7	1.384(9)
C16	C17	1.368(7)	C7	C12	1.395(9)
C23	C22	1.388(6)	C12	C11	1.385(8)
C4A	C5A	1.388(11)			

[1]1-X,1-Y,-Z

S.2.4. $[Ag_3(dppa)_3](NO_3)_2$, $9(NO_3)_2$

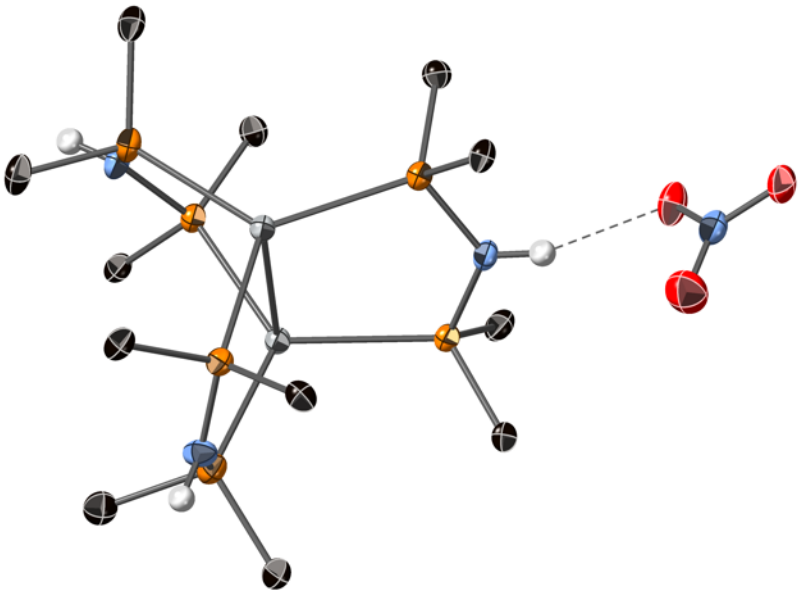

Figure S14: Solid-state structure of $\mathbf{9(NO_3)_2}$ (50% displacement ellipsoids). The complete dication was generated for clarity using a 1-X,+Y,3/2-Z symmetry operation. Only ipso carbons of the phenyl groups are depicted for clarity. Color legend: Ag (silver); P (orange); N (blue); C (black); O (red) and H (white).

Additional details for $9(NO_3)_2$: This compound crystallized in the monoclinic space group P2/c with half a molecule within the asymmetric unit. The β angle does lie suspiciously close to 90°, however, attempts to solve the structure in an orthorhombic space group were not successful. A peak of high electron density close located proximal to the silver atom was identified. This was modelled as a minor (8%) component of disorder.

Table S7: Crystal data and structure refinement for **9(NO$_3$)$_2$**.

CCDC number	1919385
Empirical formula	$C_{37}H_{33.5}AgCl_2N_2O_{1.5}P_3$
Formula weight	801.84
Temperature/K	100.01(10)
Crystal system	monoclinic
Space group	P2/c
a/Å	12.74130(10)
b/Å	12.92340(10)
c/Å	20.95380(10)
α/°	90
β/°	89.9750(10)
γ/°	90
Volume/Å^3	3450.27(4)
Z	4
ρ_{calc}g/cm^3	1.544
μ/mm^{-1}	7.706
F(000)	1630.0
Crystal size/mm^3	0.05 × 0.05 × 0.05
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.84 to 156.146
Index ranges	$-12 \leq h \leq 16$, $-16 \leq k \leq 16$, $-26 \leq l \leq 26$
Reflections collected	30543
Independent reflections	7282 [R_{int} = 0.0358, R_{sigma} = 0.0243]
Data/restraints/parameters	7282/0/431
Goodness-of-fit on F^2	1.078
Final R indexes [I>=2σ (I)]	R_1 = 0.0368, wR_2 = 0.1011
Final R indexes [all data]	R_1 = 0.0376, wR_2 = 0.1017
Largest diff. peak/hole / e Å^{-3}	0.66/-1.12

Table S8: Key bond distances of X-ray crystallography for **9(NO$_3$)$_2$**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ag1	Ag1[1]	2.8666(10)	C25	C30	1.386(5)
Ag1	P1	2.5227(14)	C36	C35	1.392(4)
Ag1	P2[1]	2.5211(9)	C3	C2	1.390(4)
Ag1	P3	2.4958(18)	C3	C4	1.372(5)
P1	N1	1.695(2)	C8	C9	1.404(4)
P1	C7	1.821(3)	C14	C15	1.380(5)
P1	C1	1.820(3)	C19	C24	1.381(5)
P1	Ag1A	2.26(2)	C19	C20	1.375(5)
P2	N1	1.673(2)	C6	C5	1.380(4)
P2	C13	1.823(3)	C5	C4	1.391(4)
P2	C19	1.823(3)	C18	C17	1.385(5)
P2	Ag1A[1]	2.381(13)	C35	C34	1.389(5)
P3	N2	1.6141(16)	C12	C11	1.383(4)
P3	C31	1.835(3)	C9	C10	1.380(5)
P3	C25	1.844(3)	C26	C27	1.381(5)
P3	Ag1A	2.98(5)	C32	C33	1.390(5)
Cl1	C37	1.769(4)	C17	C16	1.391(5)
Cl2	C37	1.761(4)	C34	C33	1.380(6)
O1	N3	1.261(3)	C30	C29	1.397(5)
N3	O2	1.226(5)	C24	C23	1.393(5)
C7	C8	1.384(4)	C16	C15	1.383(6)
C7	C12	1.397(4)	C10	C11	1.376(5)
C13	C14	1.401(4)	C28	C27	1.375(6)
C13	C18	1.396(4)	C28	C29	1.367(7)
C1	C2	1.388(4)	C22	C23	1.369(6)
C1	C6	1.399(4)	C22	C21	1.357(7)
C31	C36	1.388(4)	C20	C21	1.386(5)
C31	C32	1.395(4)	Ag1A	Ag1A[1]	2.943(16)
C25	C26	1.397(4)			

[1]1-X,+Y,3/2-Z

S.2.5. $[Ag_3Cl_2(dppa)_3](BF_4)$, $10(BF_4)$

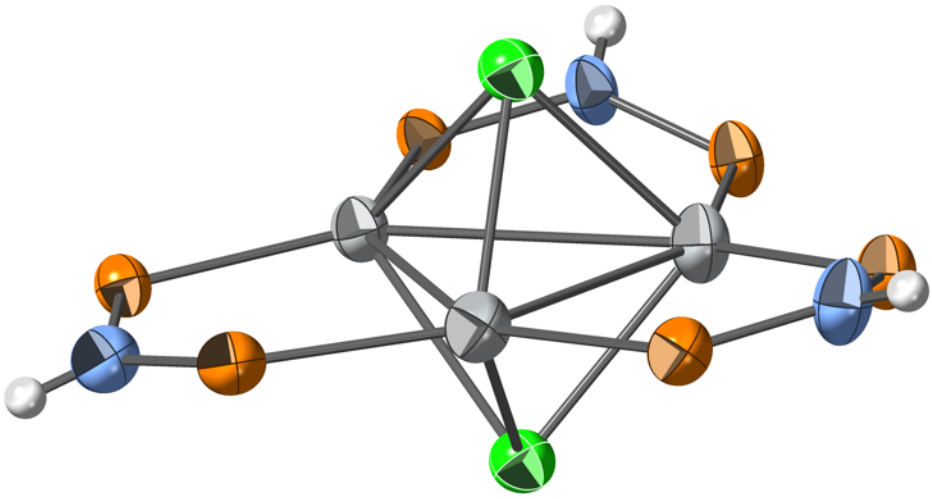

Figure S15: Solid-state structure of the cationic portion of **$10(BF_4)$** (50% displacement ellipsoids). All phenyl groups omitted for clarity. Color legend: Ag (silver); P (orange); N (blue) and H (white); and Cl (green).

Additional details for $10(BF_4)$: This compound crystallized in the monoclinic space group $P2_1$ with two independent molecules in the asymmetric unit. This compound was refined as an inversion twin, with the final twin scale factor being 0.051(9). Some phenyl groups were modelled as disordered over two sites. Two level A checkcif alerts arise due to the close proximities of some of the disordered components. Small voids (197 $Å^3$) were identified in the unit cell, each containing ca. 45 electrons. Structure factors for these electrons were generated using the solvent masking algorithm in Olex2. It is suspected that each void contains a highly disordered molecule of pentane.

Table S9: Crystal data and structure refinement for **10(BF$_4$)**.

CCDC number	1919383
Empirical formula	$C_{72}H_{63}Ag_3BCl_2F_4N_3P_6$
Formula weight	1637.39
Temperature/K	100.01(10)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	13.9166(2)
b/Å	26.4450(4)
c/Å	19.7632(3)
α/°	90
β/°	103.5346(15)
γ/°	90
Volume/Å^3	7071.37(18)
Z	4
ρ_{calc}g/cm^3	1.538
μ/mm^{-1}	9.018
F(000)	3288.0
Crystal size/mm^3	0.10 × 0.03 × 0.03
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	4.598 to 155.844
Index ranges	$-17 \leq h \leq 17$, $-30 \leq k \leq 33$, $-24 \leq l \leq 24$
Reflections collected	132667
Independent reflections	28371 [R_{int} = 0.0815, R_{sigma} = 0.0514]
Data/restraints/parameters	28371/501/1744
Goodness-of-fit on F^2	1.060
Final R indexes [I>=2σ (I)]	R_1 = 0.0565, wR_2 = 0.1516
Final R indexes [all data]	R_1 = 0.0592, wR_2 = 0.1542
Largest diff. peak/hole / e Å^{-3}	1.61/-1.64
Flack parameter	0.051(9)

Table S10: Key bond distances of X-ray crystallography for **10(BF$_4$)**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ag6	Ag4	3.2478(10)	P5	N3	1.688(9)	C63	C64	1.35(2)
Ag6	Ag5	3.2087(9)	P8	N4	1.691(10)	C91	C92	1.385(16)
Ag6	P10	2.433(3)	P8	C91	1.839(12)	C91	C96	1.379(15)
Ag6	Cl3	2.640(2)	P8	C85	1.838(12)	C112	C113	1.36(2)
Ag6	Cl4	2.746(2)	P4	N2	1.676(10)	C127	C132	1.384(15)
Ag6	P11	2.429(3)	P4	C43	1.816(10)	C19	C20	1.381(17)
Ag1	Ag3	3.2646(10)	P4	C37	1.864(11)	C97	C102	1.398(15)
Ag1	Ag2	3.2277(11)	P2	N1	1.702(10)	C50	C51	1.375(15)
Ag1	Cl2	2.665(3)	P2	C19	1.822(10)	C54	C53	1.381(16)
Ag1	Cl1	2.677(3)	P2	C13	1.84(3)	C42	C41	1.390(17)
Ag1	P1	2.428(3)	P2	C13A	1.82(6)	C42	C37	1.361(17)
Ag1	P6	2.430(3)	P1	N1	1.690(10)	C114	C113	1.396(16)
Ag4	Ag5	3.1805(10)	P1	C7	1.830(12)	C67	C68	1.387(16)
Ag4	P7	2.436(2)	P1	C1	1.821(15)	C67	C72	1.37(2)
Ag4	Cl3	2.793(3)	P6	C61	1.813(12)	C36	C31	1.367(18)
Ag4	Cl4	2.639(2)	P6	C67	1.830(11)	C36	C35	1.38(2)
Ag4	P12	2.435(3)	P6	N3	1.702(9)	C46	C45	1.40(2)
Ag3	Ag2	3.1737(10)	P11	C121	1.824(10)	C46	C47	1.359(18)
Ag3	Cl2	2.735(3)	P11	C127	1.825(10)	C44	C43	1.391(16)
Ag3	Cl1	2.643(2)	P11	N6	1.689(10)	C44	C45	1.380(16)
Ag3	P5	2.443(3)	P12	C133	1.869(13)	C92	C93	1.357(19)
Ag3	P4	2.422(3)	P12	N6	1.683(9)	C48	C43	1.396(15)
Ag2	Cl2	2.662(2)	P12	C139	1.787(15)	C48	C47	1.386(15)
Ag2	Cl1	2.725(3)	P3	C25	1.810(11)	C20	C21	1.39(2)
Ag2	P2	2.441(3)	P3	N2	1.695(9)	C22	C21	1.39(3)
Ag2	P3	2.436(3)	P3	C31	1.817(13)	C123	C124	1.407(17)
Ag5	P9	2.425(3)	F1	B1	1.398(16)	C56	C57	1.358(17)
Ag5	P8	2.428(3)	C109	C110	1.370(17)	C66	C65	1.392(18)
Ag5	Cl3	2.660(3)	C109	C114	1.392(15)	C31	C32	1.344(18)
Ag5	Cl4	2.663(2)	F3	B1	1.308(17)	C86	C85	1.373(19)

P10	C109	1.816(11)	C126	C121	1.375(16)	C86	C87	1.389(19)
P10	N5	1.690(9)	C126	C125	1.407(17)	C117	C118	1.363(17)
P10	C115	1.828(10)	C61	C62	1.408(15)	C104	C103	1.428(16)
P7	N4	1.697(10)	C61	C66	1.378(17)	C104	C105	1.39(2)
P7	C79	1.837(12)	C121	C122	1.399(14)	C103	C108	1.379(17)
P7	C73	1.787(16)	C10	C9	1.388(16)	C64	C65	1.415(18)
P7	C73A	1.97(4)	C10	C11	1.371(17)	C93	C94	1.392(19)
P9	N5	1.704(9)	C115	C116	1.379(16)	C131	C130	1.396(18)
P9	C97	1.808(12)	C115	C120	1.395(14)	C131	C132	1.372(15)
P9	C103	1.802(13)	C24	C23	1.40(2)	C30	C29	1.385(19)
P5	C49	1.828(10)	C24	C19	1.369(19)	C6	C5	1.363(19)
P5	C55	1.811(13)	C98	C97	1.390(18)	F4	B1	1.42(3)
C136	C137	1.33(2)	C98	C99	1.376(16)	C100	C99	1.34(2)
C69	C68	1.367(17)	C110	C111	1.353(19)	C100	C101	1.39(2)
C69	C70	1.37(2)	C136	C135	1.38(2)	C85	C90	1.386(19)
C129	C128	1.373(15)	C17	C16	1.38(2)	C139	C144	1.31(2)
C129	C130	1.377(19)	C18	C13	1.379(19)	C139	C140	1.39(2)
C111	C112	1.435(19)	C13	C14	1.40(2)	C135	C134	1.36(2)
C8	C7	1.387(15)	C14	C15	1.39(2)	C51	C52	1.41(2)
C8	C9	1.395(16)	C15	C16	1.39(2)	C37	C38	1.382(16)
C7	C12	1.370(16)	C14A	C13A	1.37(3)	C143	C144	1.45(2)
C12	C11	1.406(18)	C14A	C15A	1.36(3)	C143	C142	1.30(3)
C128	C127	1.397(15)	C13A	C18A	1.37(3)	F6	B2	1.27(3)
F2	B1	1.31(2)	C18A	C17A	1.35(3)	C28	C29	1.40(3)
C133	C138	1.34(2)	C17A	C16A	1.36(3)	C28	C27	1.38(3)
C133	C134	1.42(2)	C16A	C15A	1.36(3)	C57	C58	1.38(2)
C25	C30	1.40(2)	C82	C81	1.361(17)	C137	C138	1.38(2)
C25	C26	1.407(19)	C82	C83	1.354(16)	F5	B2	1.41(2)
C125	C124	1.372(19)	C81	C80	1.391(17)	C105	C106	1.39(2)
C49	C50	1.384(16)	C80	C79	1.355(15)	C35	C34	1.37(3)
C49	C54	1.393(15)	C79	C84	1.355(14)	C119	C118	1.39(2)
C122	C123	1.364(15)	C84	C83	1.368(14)	C119	C120	1.394(18)

C1	C6	1.375(19)	C76	C75	1.391(19)	C39	C38	1.338(18)
C1	C2	1.406(16)	C76	C77	1.387(18)	C87	C88	1.40(2)
C23	C22	1.31(3)	C75	C74	1.393(17)	C70	C71	1.38(3)
C40	C41	1.367(19)	C74	C73	1.378(17)	C2	C3	1.42(2)
C40	C39	1.40(2)	C73	C78	1.388(16)	C3	C4	1.33(3)
C55	C56	1.415(16)	C78	C77	1.382(16)	C142	C141	1.49(3)
C55	C60	1.432(18)	C73A	C78A	1.36(3)	C26	C27	1.401(19)
C116	C117	1.391(16)	C73A	C74A	1.37(3)	C94	C95	1.371(18)
C63	C62	1.398(18)	C78A	C77A	1.36(3)	C89	C88	1.39(3)
C71	C72	1.38(2)	C77A	C76A	1.36(3)	C89	C90	1.386(17)
F7	B2	1.49(4)	C76A	C75A	1.36(3)	C53	C52	1.33(2)
C59	C58	1.40(3)	C75A	C74A	1.36(3)	C141	C140	1.40(3)
C33	C32	1.41(2)	C5	C4	1.37(2)	C106	C107	1.39(2)
C17	C18	1.40(2)	C34	C33	1.31(3)	C96	C95	1.36(2)
C108	C107	1.40(2)	C101	C102	1.414(16)	C60	C59	1.39(2)
F8	B2	1.32(4)						

S.2.6. $[Ag_3Cl_2(dppa)_3](NO_3)$, $10(NO_3)$

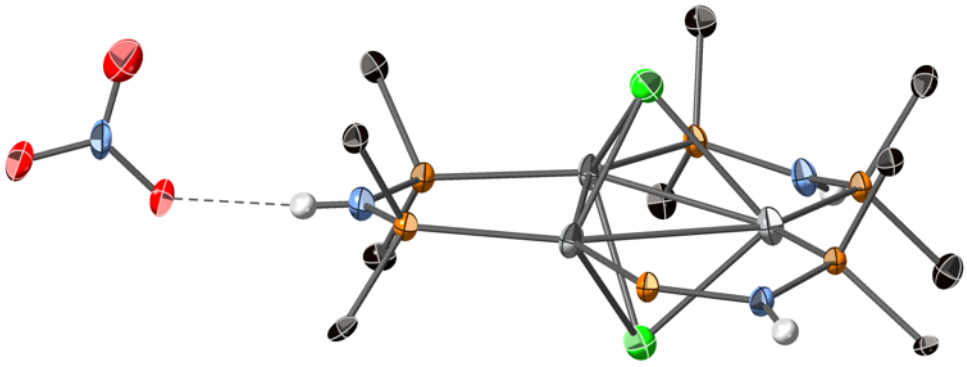

Figure S16: Solid-state structure of **$10(NO_3)$** (50% displacement ellipsoids). Only the ipso carbons of the phenyl groups are depicted for clarity. Color legend: Ag (silver); P (orange); Cl (green); N (blue); C (black); O (red) and H (white).

Additional details for $10(NO_3)$: This compound was refined as an inversion twin, with the final twin scale factor being 0.214(8). Although this compound is not chiral itself, it aggregates, due to nitrate bridging, affording a chiral packing configuration. The Friedel pairs were not collected to full coverage as determination of its absolute configuration was not of interest.

Table S11: Crystal data and structure refinement for **10(NO$_3$)**.

CCDC number	1919384
Empirical formula	$C_{72}H_{63}Ag_3Cl_2N_4O_3P_6$
Formula weight	1612.59
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	Pn
a/Å	16.0687(3)
b/Å	13.7323(2)
c/Å	16.9464(3)
α/°	90
β/°	113.932(2)
γ/°	90
Volume/Å^3	3417.91(11)
Z	2
ρ_{calc}g/cm^3	1.567
μ/mm^{-1}	9.273
F(000)	1624.0
Crystal size/mm^3	0.15 × 0.15 × 0.03
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.396 to 156.244
Index ranges	-19 ≤ h ≤ 20, -17 ≤ k ≤ 17, -21 ≤ l ≤ 17
Reflections collected	46623
Independent reflections	10797 [R_{int} = 0.0486, R_{sigma} = 0.0332]
Data/restraints/parameters	10797/2/812
Goodness-of-fit on F^2	1.067
Final R indexes [I>=2σ (I)]	R_1 = 0.0381, wR_2 = 0.1017
Final R indexes [all data]	R_1 = 0.0388, wR_2 = 0.1029
Largest diff. peak/hole / e Å^{-3}	1.09/-1.22
Flack parameter	0.214(8)

Table S12: Key bond distances of X-ray crystallography for **10(NO$_3$)**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ag1	Ag2	3.1870(6)	N4	O2	1.252(11)	C31	C32	1.401(11)
Ag1	Ag3	3.1952(7)	N4	O3	1.231(11)	C35	C34	1.383(15)
Ag1	P6	2.4457(16)	C13	C18	1.386(10)	C30	C29	1.373(11)
Ag1	P1	2.4431(18)	C19	C24	1.402(11)	C16	C17	1.399(14)
Ag1	Cl1	2.700(2)	C19	C20	1.391(11)	C51	C50	1.389(12)
Ag1	Cl2	2.6492(19)	C55	C60	1.390(11)	C51	C52	1.386(14)
Ag2	Ag3	3.2490(7)	C55	C56	1.404(11)	C61	C66	1.395(9)
Ag2	P2	2.4540(18)	C60	C59	1.387(11)	C70	C69	1.393(13)
Ag2	Cl1	2.784(2)	C67	C72	1.409(10)	C6	C5	1.371(11)
Ag2	P3	2.4460(18)	C67	C68	1.381(11)	C48	C43	1.396(11)
Ag2	Cl2	2.6609(19)	C15	C16	1.385(12)	C48	C47	1.375(12)
Ag3	P5	2.4333(16)	C62	C63	1.386(11)	C69	C68	1.392(12)
Ag3	P4	2.4331(18)	C62	C61	1.391(11)	C50	C49	1.395(11)
Ag3	Cl1	2.6578(19)	C2	C3	1.407(11)	C17	C18	1.379(12)
Ag3	Cl2	2.776(2)	C2	C1	1.379(10)	C49	C54	1.389(10)
P6	C67	1.822(8)	C7	C8	1.377(11)	C34	C33	1.403(16)
P6	N3	1.687(6)	C7	C12	1.385(11)	C5	C4	1.389(13)
P6	C61	1.834(7)	C26	C27	1.395(11)	C64	C65	1.389(13)
P5	C55	1.833(7)	C26	C25	1.398(10)	C10	C9	1.403(13)
P5	N3	1.704(6)	C27	C28	1.364(12)	C10	C11	1.387(14)
P5	C49	1.820(7)	C72	C71	1.368(11)	C22	C21	1.370(13)
P4	N2	1.683(6)	C24	C23	1.384(11)	C22	C23	1.399(14)
P4	C37	1.842(8)	C37	C38	1.403(12)	C43	C44	1.393(11)
P4	C43	1.818(8)	C37	C42	1.384(12)	C52	C53	1.399(13)
P1	C7	1.838(8)	C20	C21	1.383(11)	C54	C53	1.383(12)
P1	N1	1.681(6)	C3	C4	1.367(12)	C57	C56	1.389(11)
P1	C1	1.834(7)	C63	C64	1.413(11)	C40	C41	1.395(17)
P2	C13	1.835(8)	C1	C6	1.416(9)	C40	C39	1.377(15)
P2	C19	1.831(8)	C28	C29	1.400(12)	C8	C9	1.386(13)
P2	N1	1.687(6)	C38	C39	1.391(14)	C44	C45	1.385(13)

P3	N2	1.685(7)	C25	C30	1.405(11)	C12	C11	1.373(13)
P3	C25	1.820(7)	C71	C70	1.383(13)	C33	C32	1.377(13)
P3	C31	1.835(8)	C58	C59	1.395(13)	C66	C65	1.384(11)
O1	N4	1.266(10)	C58	C57	1.373(12)	C45	C46	1.395(15)
C14	C13	1.380(11)	C36	C31	1.387(13)	C42	C41	1.385(15)
C14	C15	1.397(11)	C36	C35	1.399(12)	C47	C46	1.370(15)

S.3. DFT Studies

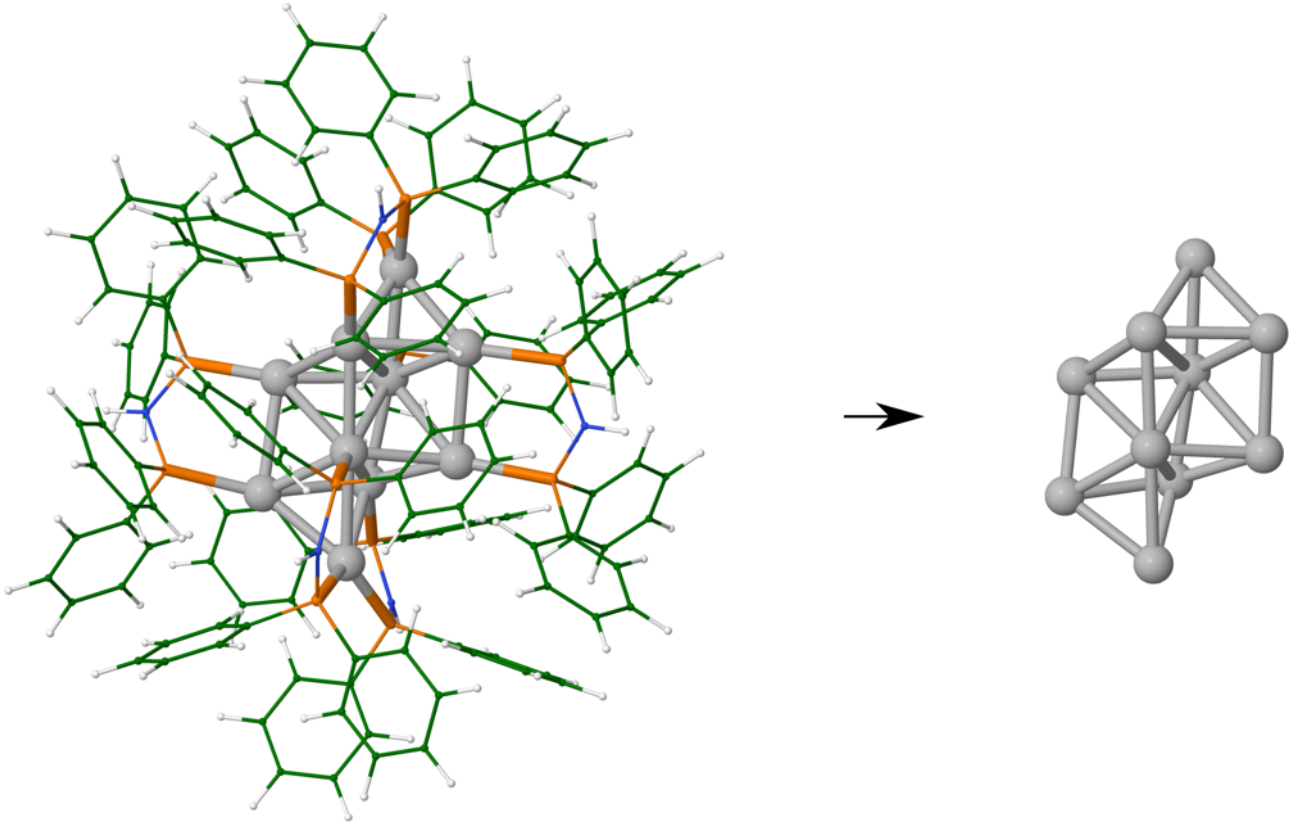

Figure S17: Fully optimized structure of $[Ag_{10}(dppa)_6]^{2+}$. The Ag_{10} cluster core is depicted on the right. Color legend: Ag (silver); P (orange); N (blue); H (white) and C (green).

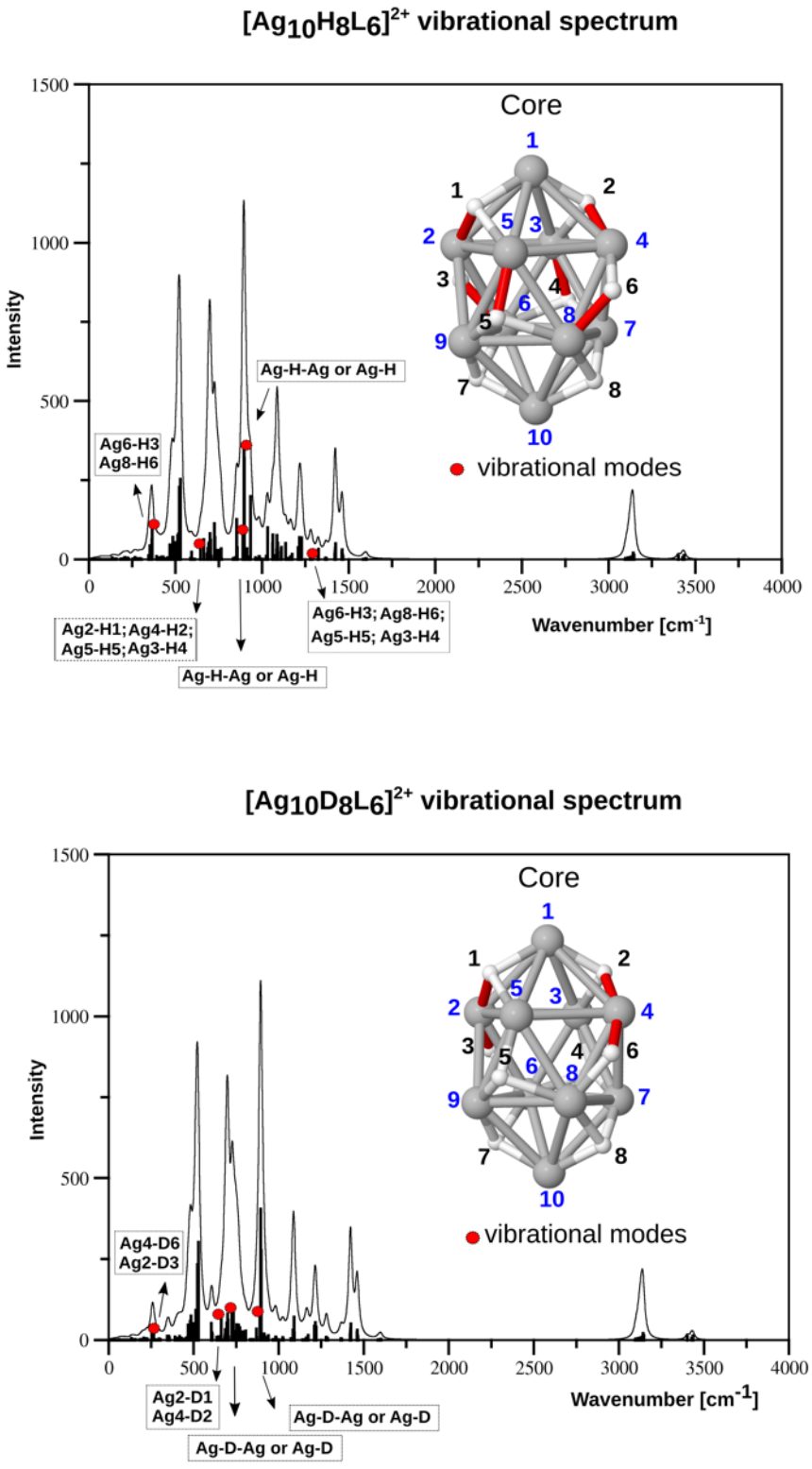

Figure S18: Predicted IR spectra analyses of $[Ag_{10}H_8(dppa)_6]^{2+}$ (top) and $[Ag_{10}D_8(dppa)_6]^{2+}$ (bottom). Red spots are assigned to stretching and bending modes of Ag-H or Ag-D. Selection has been made according to the range of intensity (KM/mole).

S.4. Ion Mobility Mass Spectrometry

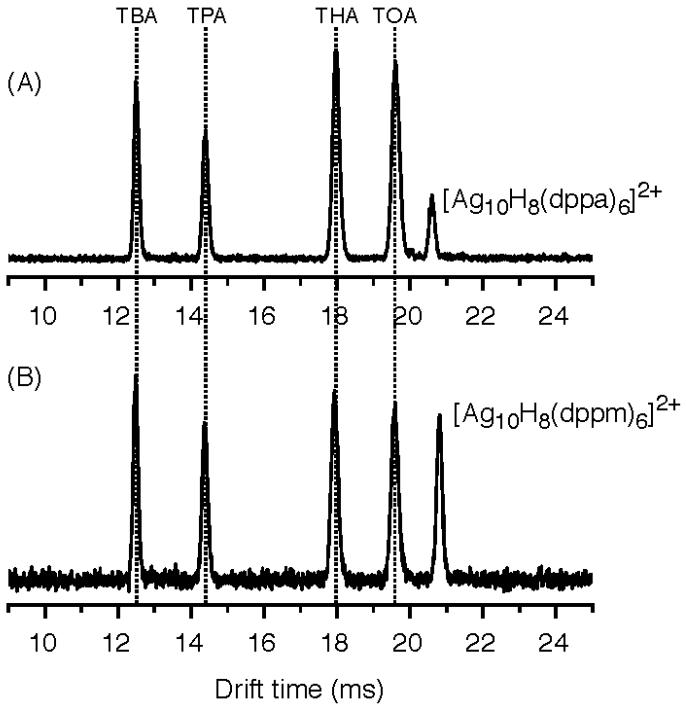

Figure S19: Arrival time distributions used to determine collision cross section values for (A) $\mathbf{7}^{2+}$ and (B) $\mathbf{4}^{2+}$; TBA = tetrabutylammonium, TPA = tetrapentylammonium, THA= tetraheptylammonium, TOA = tetraoctylammonium.

S.5. Multistage Mass Spectrometry

Modified Q Exactive Orbitrap mass spectrometer

193 nm UVPD MS/MS experiments were conducted on a modified Q Exactive Orbitrap mass spectrometer similar to that described by Fort and co-workers and which has been described elsewhere.[S1] Briefly, a CaF_2 optical window was introduced into the rear access port of the vacuum manifold. After removal of the electrometer positioned at the exit of the HCD cell, the output from a Coherent ExciStar XS ArF excimer laser (Santa Clara, CA, USA) (8 mg energy max., up to 500 Hz rep. rate, 2.5 W average pulse power, 5 ns pulse duration) was directed coaxially into the HCD cell using standard UV optics. Collimation of the laser pulses was achieved using an aperture plate with a 2.0 mm central hole mounted inside the vacuum manifold between the optical window and the HCD cell. The laser was triggered by using the output from the split lens of the mass spectrometer. Control over the ion trapping time, and the HCD collision energy (i.e., below the default value of 10% NCE), was achieved using custom software patches within the mass spectrometer control software.

Modified LTQ mass spectrometer

The LTQ mass spectrometer was modified to allow the introduction of a laser beam into the ion trap. The posterior plate of the LTQ was modified with a quartz window to transmit 266 nm laser pulses from a Nd:YAG laser (Quantel Big Sky). Pulses were triggered externally from a pulse generator (HP8116A Pulse/Function Generator 50 MHz) to synchronize with the desired MS^n activation step. Multiphoton excitation of the ions *in vacuo* causes fragmentation.

Mass spectrometry details

Silver cation complexes of $[Ag_{10}H_8(dppa)_6]^{2+}$, $\mathbf{7^{2+}}$, $[Ag_{10}D_8(dppa)_6]^{2+}$, $\mathbf{7_D^{2+}}$, $[Ag_{10}H_8(dppm)_6]^{2+}$, $\mathbf{4^{2+}}$, were introduced into the mass spectrometer as 10 – 100 μM acetonitrile solutions. For samples introduced into the LTQ mass spectrometer; the syringe pump was set at a flow rate of 5 – 10 μL min^{-1}. The electrospray conditions were tuned for optimal signal intensity of the target ions. Typical parameters were as follows: spray voltage, 2.5 – 5.0 kV; capillary temperature, 250 °C; nitrogen

sheath gas pressure, 10 (arbitrary units); capillary voltage, 10 – 25 V; and tube lens voltage, 120 – 130 V. For unimolecular fragmentation reactions of $\mathbf{7}^{2+}$, CID-MS/MS was employed. A mass selection window of 10-15 *m/z* was used to isolate the full range of carbon and silver isotopes. The mass-selected precursor ion was typically depleted to 10-20% using a normalized collision energy typically between 15-25% with an activation Q value of 0.25 and an activation time of 30 ms was typically used to acquire spectra.

Samples introduced into the Orbitrap Fusion Lumos mass spectrometer via nanoESI (nESI) using an Advion Triversa Nanomate (Advion, Ithaca, NY, USA) operating at a spray voltage of 1.2 kV and a gas pressure of 0.3 psi. The ion source interface settings (inlet temperature of 200 °C and S-Lens value of 50%) were optimized to maximize the sensitivity of the precursor ions while minimizing in-source fragmentation. All nESI spectra were acquired in the Orbitrap mass (heated capillary temperature = 200 °C, RF lens set at 40 %). MS spectra were acquired from *m/z* 350-2000 to observe the range of silver cationic complexes formed initially before acquiring from *m/z* 1600-2000 to focus on samples of $\mathbf{7}^{2+}$, $\mathbf{7_D}^{2+}$ and $\mathbf{4}^{2+}$, at a mass resolving power of 500,000 and an AGC target at 4.0×10^5. For MS^n experiments, monoisotopic precursor ions were mass selected using the isolation quadrupole (± 0.2 *m/z*), then subjected to ion trap CID using an activation Q value of 0.25 and an activation time of 10 ms or to HCD-MS/MS by the collision cell where the collision energies were individually optimized for fragment ion efficiency.

For samples of $\mathbf{7}^{2+}$, $\mathbf{7_D}^{2+}$ and $\mathbf{4}^{2+}$ that were introduced into the modified Q Exactive Orbitrap mass spectrometer via electrospray ionization (ESI); the syringe pump was set at a flow rate of 10 μL/min, using a spray voltage of 3.5 kV, heated capillary temperature of 200 °C, a sheath gas pressure of 5, and RF lens set at 50%. For HCD-MS/MS experiments collected on this instrument, mass-selection of precursor ions were conducted using the isolation quadrupole (± 10 *m/z* to collect the full isotopic envelope of the silver clusters), then subjected to tandem mass spectrometry using a range of collision energies.

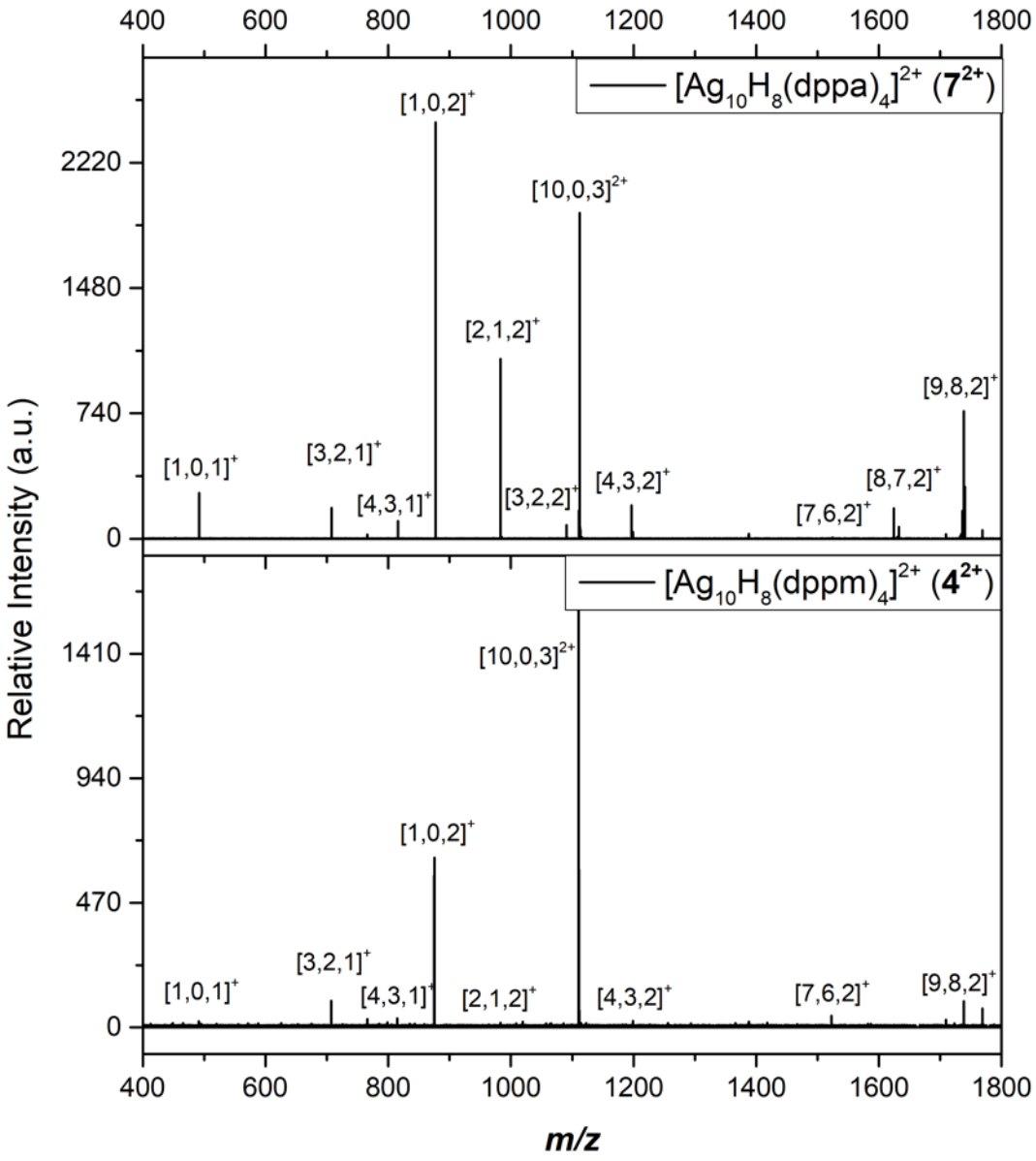

Figure S20: Single isotope multistage mass spectrometry low energy CID experiments. Top: MS^3 spectra on $[Ag_{10}H_8(dppa)_4]^{2+}$ mass-selected precursor ion, obtained using a Q value of 0.25, an activation time of 10 ms and the normalized collision energy (NCE) 30%. Bottom: MS^3 spectra on $[Ag_{10}H_8(dppm)_4]^{2+}$ mass-selected precursor ion, obtained using a Q value of 0.25, an activation time of x ms and NCE 26%. The numbers in the square brackets represent the stoichiometry of silver atoms, hydrogen atoms and ligands, e.g., $[3,2,1]^+ = [Ag_3H_2(L)_1]^+$. The following monoisotopic ions are not observed: $[2,1,1]^+$, $[3,2,2]^+$ (for dppm), $[6,5,2]^+$. Note that for the fragment ions of $[Ag_{10}H_8(dppa)_4]^{2+}$, spontaneous H_2 loss is observed involving one H atom of the ligand. These related species are not illustrated here for the simplicity of comparison.

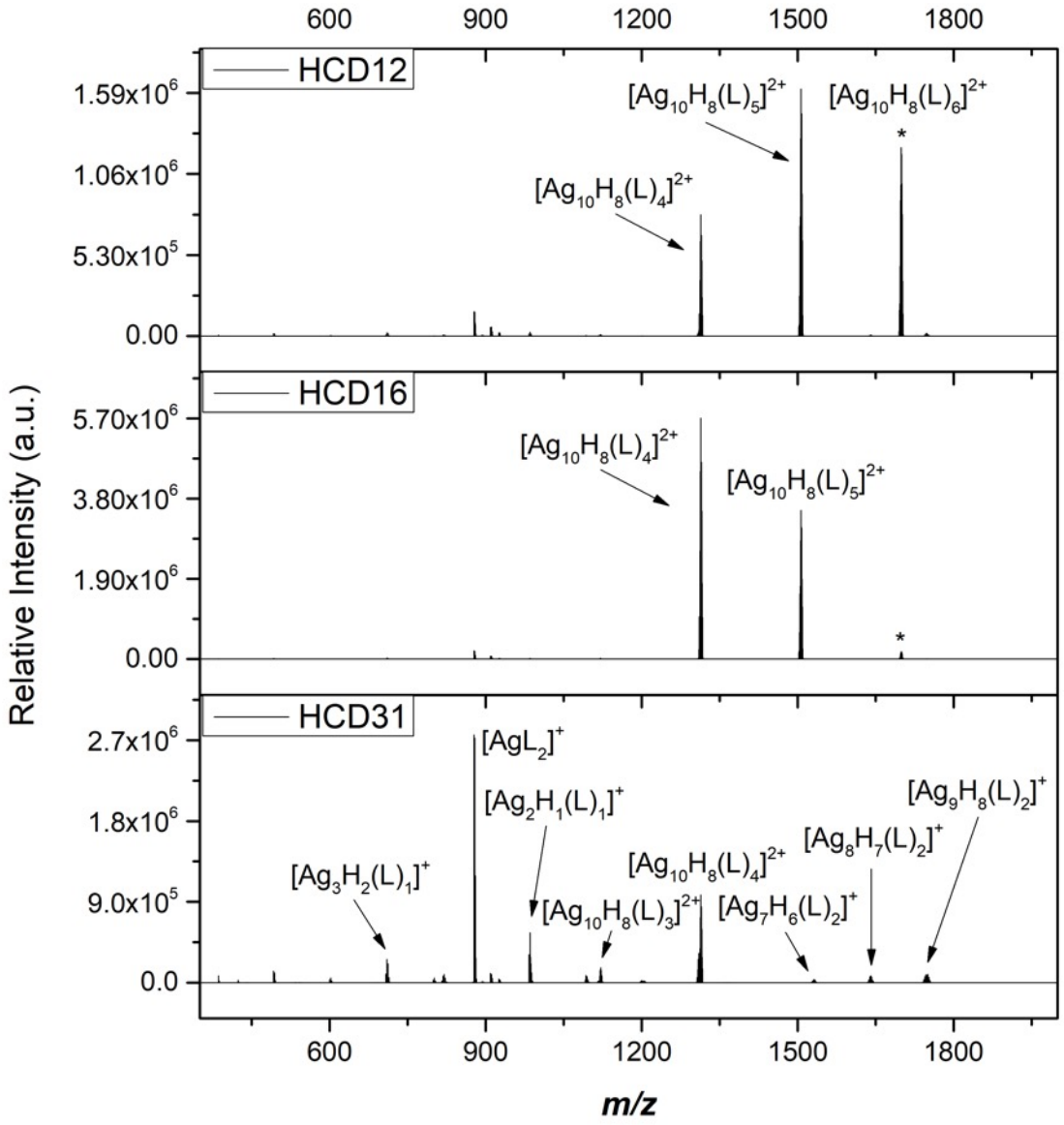

Figure S21: HCD-MS/MS of $[Ag_{10}H_8(dppa)_6]^{2+}$ ($\mathbf{7^{2+}}$) mass-selected precursor ion recorded on a Q Exactive Orbitrap mass spectrometer. Spectra acquired at varying collision energies as indicated by each frame. (*) represents mass-selected precursor ion.

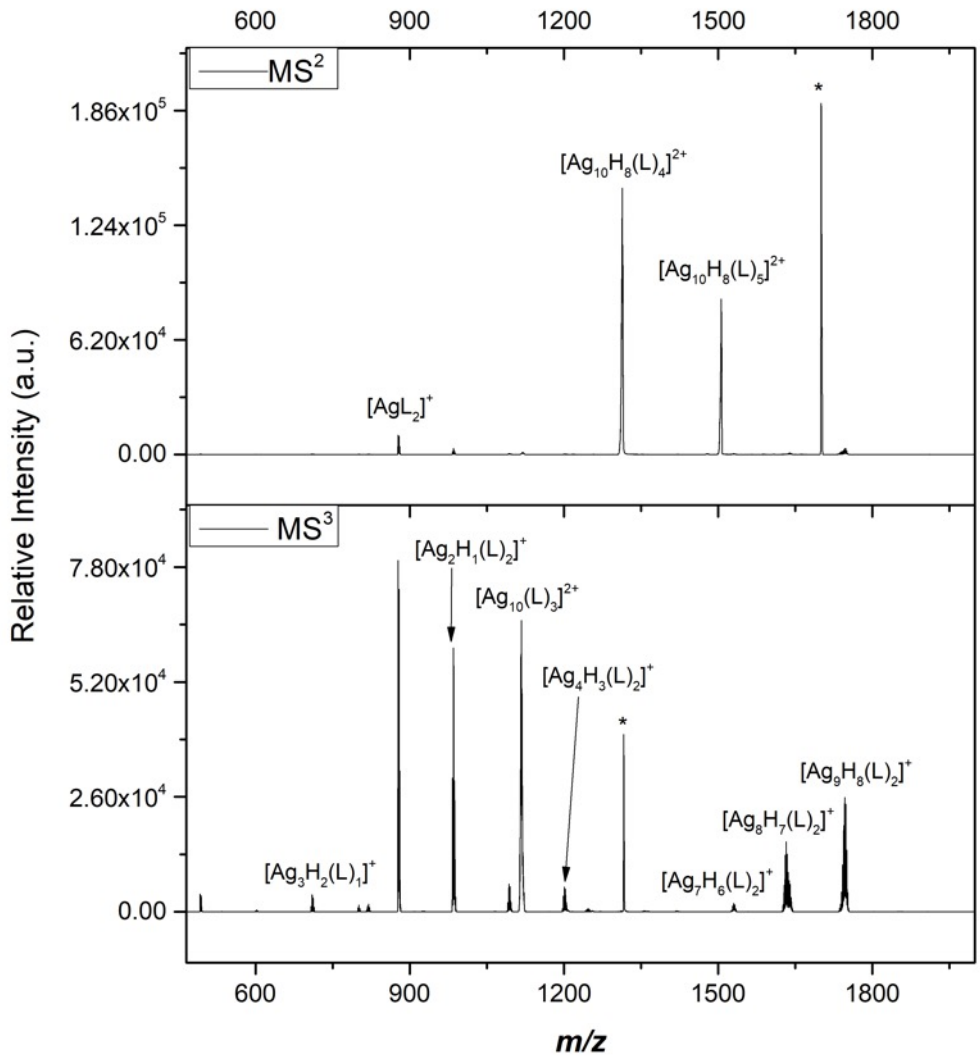

Figure S22: Multistage mass spectrometry lower energy CID LTQ experiments. MS^2 (top panel) of $[Ag_{10}H_8(dppa)_6]^{2+}$ (**7**$^{2+}$) showing sequential ligand loss, obtained using a Q value of 0.25, an activation time of 30 ms and the normalized collision energy (NCE) 18% and; MS^3 (bottom panel) of the daughter ion of **7**$^{2+}$, $[Ag_{10}H_8(dppa)_4]^{2+}$, revealing its unimolecular fragmentation pattern, obtained using a Q value of 0.25, an activation time of 30 ms and NCE 25%.

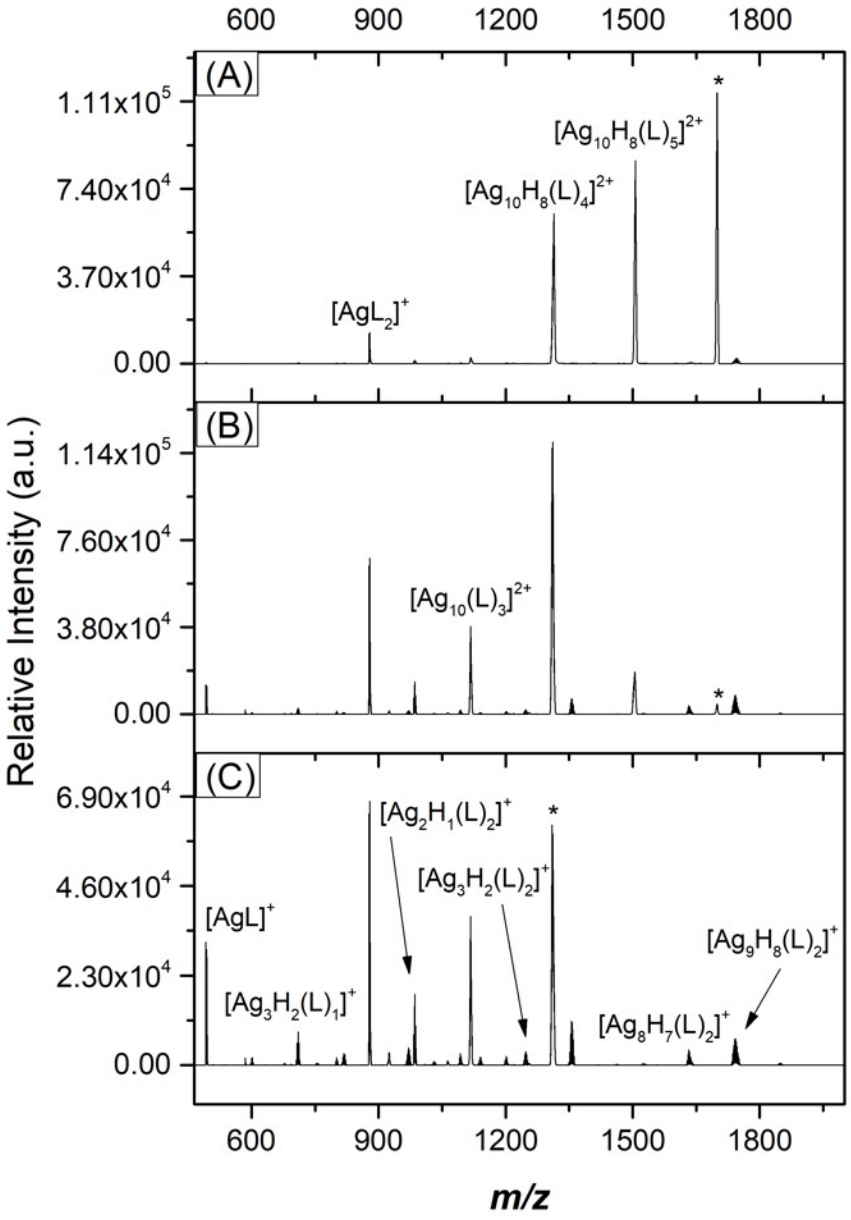

Figure S23: LID LTQ mass spectra at 266 nm of (A) $[Ag_{10}H_8(dppa)_6]^{2+}$ ($\mathbf{7^{2+}}$) at 200 ms; (B) $\mathbf{7^{2+}}$ at 500 ms; (C) CID-MS/MS of $\mathbf{7^{2+}}$ followed by isolation of $[Ag_{10}H_8(dppa)_4]^{2+}$ and subsequent LID at 90 ms.

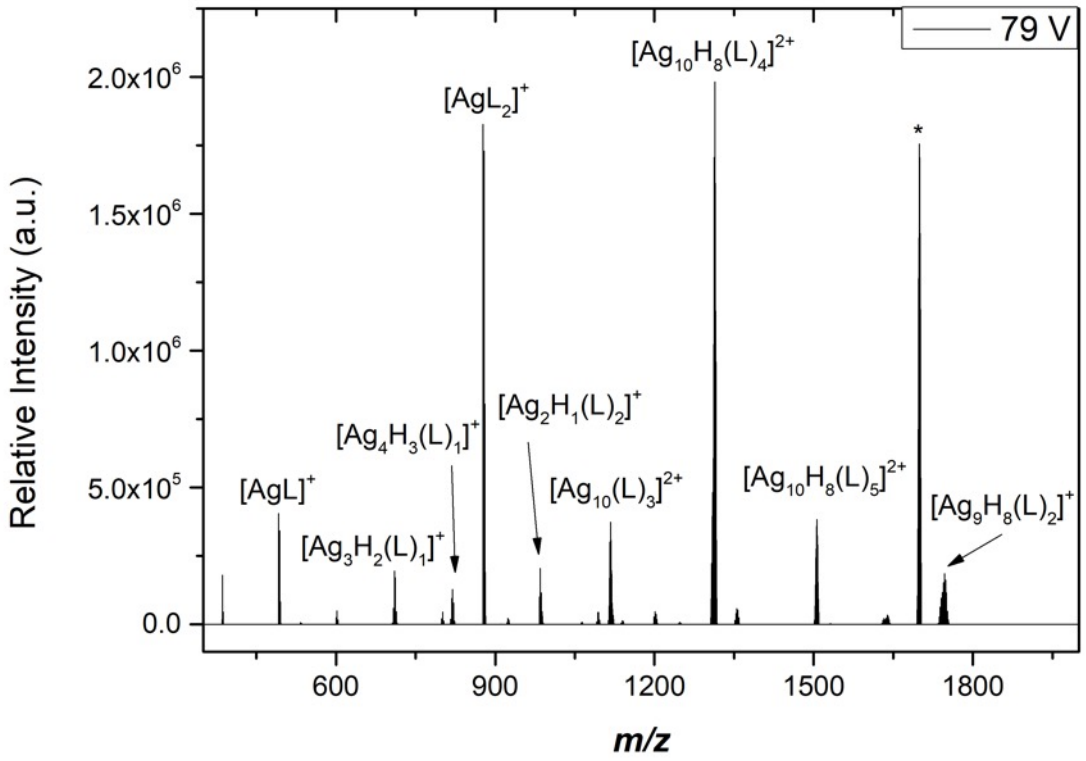

Figure S24: 193 nm UVPD of $[Ag_{10}H_8(dppa)_6]^{2+}$ (**7**$^{2+}$) as the mass-selected precursor ion recorded on a Q Exactive Orbitrap mass spectrometer. (*) represents the mass-selected precursor ion.

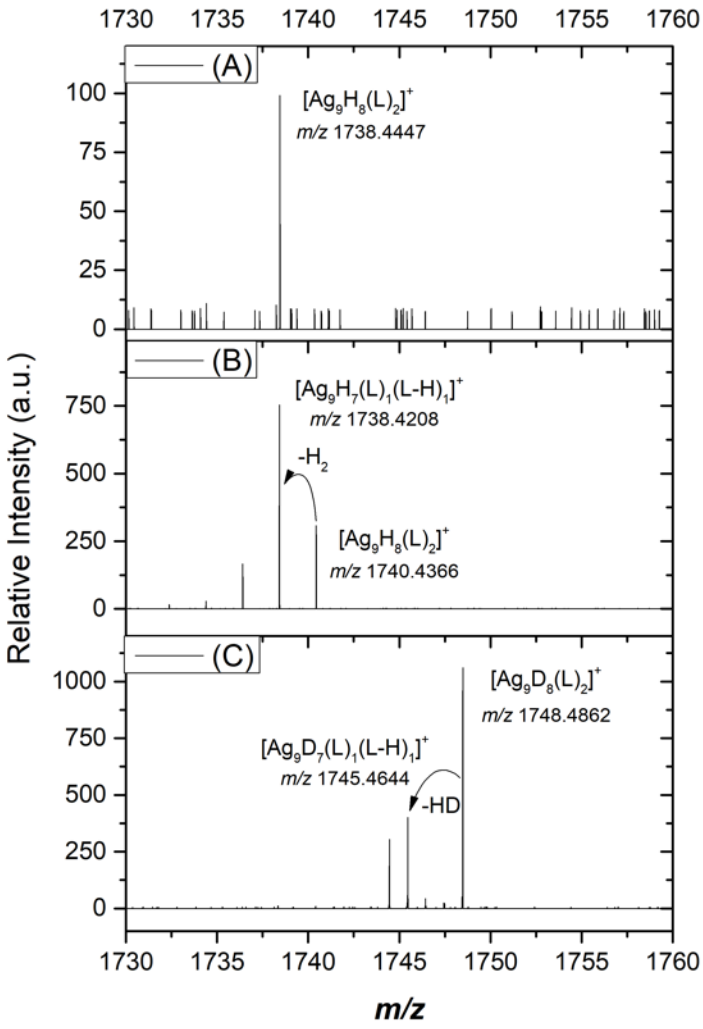

Figure S25: Single isotope multistage mass spectrometry low energy CID experiments highlighting the more labile dppa ligand through observed HD losses; (A) MS^3 of $[Ag_{10}H_8(L)_4]^{2+}$, L = dppm = bis(diphenylphosphino)methane, to give $[Ag_9H_8(L)_2]^+$ (*m/z* 1738.4447) and its complementary ion pair $[Ag(L)_2]^+$ (*m/z* 877.1344, not shown); (B) MS^3 of $[Ag_{10}H_8(L)_4]^{2+}$, L = dppa = bis(diphenylphosphino)amine, to give $[Ag_9H_8(L)_2]^+$ (*m/z* 1740.4366) which subsequently undergoes spontaneous H_2 loss to give $[Ag_9H_7(L)(L\text{-}H)]^+$ (*m/z* 1738.4208). $[Ag_{10}D_8(L)_3]^{2+}$ → $[Ag_2D_1(dppa)_1]^+$ → $[Ag_2(dppa\text{-}H)]^+$ + HD is a representative reaction of HD loss involving the dppa ligand.

Table S13: Ions formed from HCD-MS/MS of $\mathbf{7}^{2+}$ illustrating the sequential liberation of H_2. Experimental and theoretical accurate mass.

Ion	Molecular Formula	Monoisotopic mass - calculated (m/z)	Monoisotopic mass - experimental (m/z)	Mass error (ppm)
$[Ag_{10}H_8(L)_3]^{2+}$	$C_{72}H_{71}Ag_{10}N_3P_6^{+2}$	1116.22862	1116.2284	-0.197092241
$[Ag_{10}H_6(L)_3]^{2+}$	$C_{72}H_{69}Ag_{10}N_3P_6^{+2}$	1115.2208	1115.2204	-0.358673368
$[Ag_{10}H_4(L)_3]^{2+}$	$C_{72}H_{67}Ag_{10}N_3P_6^{+2}$	1114.21297	1114.2128	-0.152574063
$[Ag_{10}H_2(L)_3]^{2+}$	$C_{72}H_{65}Ag_{10}N_3P_6^{+2}$	1113.20515	1113.2049	-0.224576755
$[Ag_{10}H_0(L)_3]^{2+}$	$C_{72}H_{63}Ag_{10}N_3P_6^{+2}$	1112.19732	1112.1971	-0.197806627
$[Ag_{10}H_7(L)_3]^{2+}$	$C_{72}H_{70}Ag_{10}N_3P_6^{+2}$	1115.7247	not observed	
$[Ag_{10}H_5(L)_3]^{2+}$	$C_{72}H_{68}Ag_{10}N_3P_6^{+2}$	1114.71689	1114.7143	-2.32346
$[Ag_{10}H_3(L)_3]^{2+}$	$C_{72}H_{66}Ag_{10}N_3P_6^{+2}$	1113.70906	1113.7052	-3.465896
$[Ag_{10}H_1(L)_3]^{2+}$	$C_{72}H_{64}Ag_{10}N_3P_6^{+2}$	1112.70124	1112.7011	-0.12582
$[Ag_{10}D_8(L)_3]^{2+}$	$C_{72}H_{63}[^2H]_8Ag_{10}N_3P_6^{+2}$	1120.25373	1120.2531	-0.562372598
$[Ag_{10}D_6(L)_3]^{2+}$	$C_{72}H_{63}[^2H]_6Ag_{10}N_3P_6^{+2}$	1118.23963	1118.2385	-1.01051686
$[Ag_{10}D_4(L)_3]^{2+}$	$C_{72}H_{63}[^2H]_4Ag_{10}N_3P_6^{+2}$	1116.22553	1116.2253	-0.206051549
$[Ag_{10}D_2(L)_3]^{2+}$	$C_{72}H_{63}[^2H]_2Ag_{10}N_3P_6^{+2}$	1114.21143	1114.2109	-0.475672737
$[Ag_{10}D_8(L)_3]^{2+}$ -H*	$C_{72}H_{62}[^2H]_8Ag_{10}N_3P_6^{+2}$	1119.74982	1119.7502	0.339361519
$[Ag_{10}D_6(L)_3]^{2+}$ -H*	$C_{72}H_{62}[^2H]_6Ag_{10}N_3P_6^{+2}$	1117.73572	1117.7365	0.697839378
$[Ag_{10}D_4(L)_3]^{2+}$ -H*	$C_{72}H_{62}[^2H]_4Ag_{10}N_3P_6^{+2}$	1115.72161	1115.7217	0.080665284
$[Ag_{10}D_2(L)_3]^{2+}$ -H*	$C_{72}H_{62}[^2H]2Ag_{10}N_3P_6^{+2}$	1113.70751	1113.7096	1.876614803
$[Ag_{10}D_8(L)_3]^{2+}$ -D*	$C_{72}H_{63}[^2H]_7Ag_{10}N_3P_6^{+2}$	1119.24668	not observed	
$[Ag_{10}D_6(L)_3]^{2+}$ -D*	$C_{72}H_{63}[^2H]5Ag_{10}N_3P_6^{+2}$	1117.23258	1117.2248	-6.963635092
$[Ag_{10}D_4(L)_3]^{2+}$ -D*	$C_{72}H_{63}[^2H]3Ag_{10}N_3P_6^{+2}$	1115.21848	1115.2171	-1.237425693
$[Ag_{10}D_2(L)_3]^{2+}$ -D*	$C_{72}H_{63}[^2H]1Ag_{10}N_3P_6^{+2}$	1113.20437	1113.2036	-0.691696889
$[Ag_{10}D_8(L)_3]^{2+}$ -HD	$C_{72}H_{62}[^2H]_7Ag_{10}N_3P_6^{+2}$	1118.74277	1118.7411	-1.492747077
$[Ag_{10}D_6(L)_3]^{2+}$ -HD	$C_{72}H_{62}[^2H]_5Ag_{10}N_3P_6^{+2}$	1116.72867	1116.7275	-1.04770302
$[Ag_{10}D_4(L)_3]^{2+}$ -HD	$C_{72}H_{62}[^2H]3Ag_{10}N_3P_6^{+2}$	1114.71456	1114.7134	-1.040625144
$[Ag_{10}D_2(L)_3]^{2+}$ -HD	$C_{72}H_{62}[^2H]Ag_{10}N_3P_6^{+2}$	1112.70046	1112.7001	-0.323537208

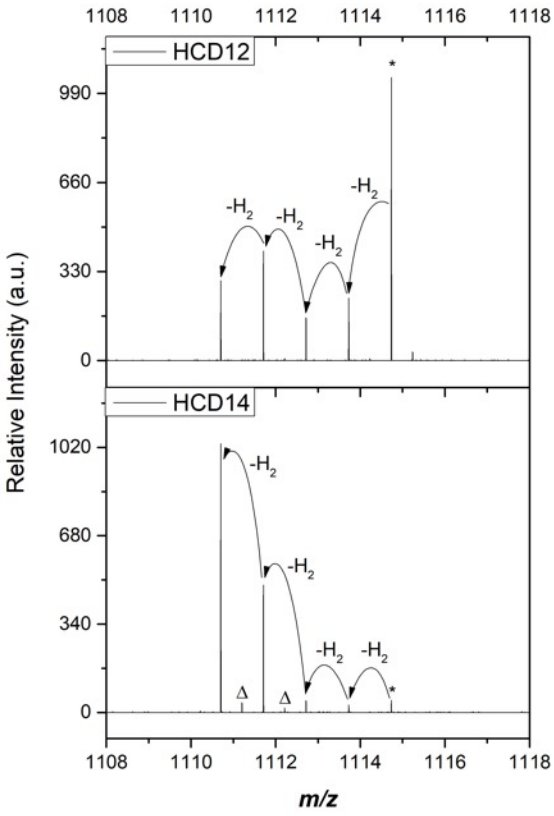

Figure S26: HCD-MS/MS of $[Ag_{10}H_8(dppm)_6]^{2+}$ (**4**$^{2+}$) as the mass-selected precursor ion recorded on a Q Exactive Orbitrap mass spectrometer. The fragmentation pattern illustrating sequential liberation of H_2 to form $[Ag_{10}(dppm)_3]^{2+}$ (m/z 1110.7039 (exp)/m/z 1114.7044 (calc)) via the metastable $[Ag_{10}H_8(dppm)_3]^{2+}$ (m/z 1114.7354 (exp)/m/z 1114.7457 (calc)). Δ = *m/z* -H, loss of proton.

S.6. Gaussian Cartesian Coordinates For Isomers $7a^{2+}$ and $7b^{2+}$ of $[Ag_{10}H_8(dppa)_6]^{2+}$ (Figure 3C and S18) and $[Ag_{10}(dppa)_6]^{2+}$(Figure S17)

Table S14: Cartesian coordinates for **$7a^{2+}$**.

C	5.166577	-2.046687	2.553848
C	5.322141	-3.025308	1.550728
C	5.651698	-4.345503	1.892390
C	5.803961	-4.704104	3.241552
C	5.620583	-3.740066	4.247833
C	5.302606	-2.415551	3.908381
P	4.836228	-0.317310	2.015842
C	6.523372	0.409152	1.851584
C	7.702255	-0.359506	1.817362
C	8.946904	0.273509	1.664898
C	9.024372	1.668828	1.538313
C	7.848624	2.439687	1.564377
C	6.604367	1.814844	1.720604
Ag	3.390861	-0.000025	0.000002
P	4.836021	0.317197	-2.015929
C	5.166340	2.046358	-2.554616
C	5.322952	3.025200	-1.551869
C	5.652331	4.345271	-1.894167
C	5.803450	4.703519	-3.243555
C	5.619106	3.739241	-4.249424
C	5.301225	2.414856	-3.909360
Ag	1.217523	0.817168	1.856251
P	2.726645	1.045983	3.798984
C	2.956372	2.775539	4.375345
C	1.799365	3.578076	4.473100
C	1.894409	4.895456	4.944684
C	3.141084	5.427867	5.312670
C	4.298084	4.638678	5.201790
C	4.209160	3.318524	4.730459
Ag	1.216861	-0.817543	-1.856248
P	2.726373	-1.046439	-3.798849
C	2.956109	-2.775887	-4.375512
C	4.208871	-3.318672	-4.731067
C	4.297797	-4.638641	-5.202905
C	3.140822	-5.427867	-5.313849
C	1.894197	-4.895688	-4.945388
C	1.799151	-3.578479	-4.473314
Ag	1.322717	1.962344	-0.793713
P	1.220009	4.462841	-0.873284
C	1.170234	5.114304	-2.593278
C	0.193228	6.023913	-3.044408
C	0.234209	6.502419	-4.365339
C	1.241091	6.069987	-5.244103
C	2.202561	5.143126	-4.802898
C	2.165110	4.660390	-3.487469
Ag	1.322928	-1.962217	0.793960

P	1.219799	-4.462814	0.873376
C	1.170521	-5.114147	2.593439
C	0.193831	-6.023969	3.044822
C	0.235227	-6.502426	4.365758
C	1.242190	-6.069704	5.244289
C	2.203320	-5.142601	4.802847
C	2.165468	-4.659939	3.487403
N	-0.055865	-5.288043	0.049212
P	-1.548952	-4.610178	-0.490256
C	-1.885686	-5.585509	-2.009216
C	-0.881676	-6.327751	-2.664804
C	-1.188249	-7.048735	-3.831726
C	-2.487205	-7.021054	-4.364018
C	-3.481852	-6.253504	-3.731744
C	-3.185047	-5.536134	-2.564696
C	2.677569	-5.332592	0.152096
C	3.153769	-6.559925	0.659232
C	4.222536	-7.214852	0.026390
C	4.826547	-6.644703	-1.107253
C	4.357217	-5.419411	-1.611983
C	3.284843	-4.764308	-0.987875
Ag	-1.258786	-2.115292	-0.774107
Ag	-1.192417	0.696935	-1.761863
P	-2.464126	0.088692	-3.803236
C	-2.723355	1.572027	-4.869140
C	-3.817118	1.701139	-5.751674
C	-3.950870	2.849097	-6.546881
C	-2.987419	3.871411	-6.477661
C	-1.898956	3.751455	-5.599849
C	-1.772314	2.610883	-4.790666
Ag	-3.337447	-0.000121	0.000009
P	-4.799202	0.591668	1.918722
C	-5.541906	2.270858	1.809356
C	-5.408065	2.974246	0.595586
C	-6.006785	4.234081	0.433284
C	-6.722849	4.809594	1.493906
C	-6.848485	4.120893	2.714942
C	-6.270123	2.852686	2.870915
Ag	-1.192155	-0.695573	1.761996
P	-2.464372	-0.088788	3.803465
C	-2.723281	-1.572305	4.869162
C	-1.772236	-2.611119	4.790225
C	-1.898533	-3.751762	5.599357
C	-2.986650	-3.871831	6.477584
C	-3.950111	-2.849559	6.547271
C	-3.816696	-1.701524	5.752115
Ag	-1.259184	2.115595	0.774568
P	-1.548319	4.610360	0.490755
C	-1.885290	5.585654	2.009692
C	-0.881464	6.328083	2.665331
C	-1.188261	7.049046	3.832210
C	-2.487263	7.021160	4.364375
C	-3.481733	6.253440	3.732026

C	-3.184700	5.536081	2.565029
P	-4.799125	-0.591814	-1.918638
C	-5.541983	-2.270930	-1.809289
C	-5.408427	-2.974225	-0.595438
C	-6.007347	-4.233965	-0.433130
C	-6.723315	-4.809466	-1.493816
C	-6.848659	-4.120859	-2.714939
C	-6.270102	-2.852747	-2.870928
N	-4.036266	-0.534771	-3.462743
C	-1.859297	-1.179655	-4.986297
C	-1.131873	-0.831550	-6.142961
C	-0.669073	-1.835139	-7.008599
C	-0.920360	-3.186636	-6.726197
C	-1.633188	-3.537813	-5.567287
C	-2.096904	-2.542055	-4.696507
N	-4.036611	0.534420	3.462946
C	-1.859670	1.179524	4.986582
C	-1.132110	0.831436	6.143169
C	-0.669123	1.835057	7.008673
C	-0.920358	3.186549	6.726208
C	-1.633320	3.537704	5.567371
C	-2.097226	2.541915	4.696728
C	-6.254082	0.511989	-2.145054
C	-7.540106	0.171506	-1.678534
C	-8.587496	1.103762	-1.763058
C	-8.363139	2.376151	-2.311998
C	-7.083291	2.717127	-2.783206
C	-6.033386	1.793083	-2.698588
C	-6.254261	-0.512042	2.144794
C	-7.540061	-0.171556	1.677652
C	-8.587529	-1.103750	1.761827
C	-8.363488	-2.376069	2.311060
C	-7.083874	-2.717035	2.782907
C	-6.033877	-1.793060	2.698623
C	-2.776132	-5.272078	0.726027
C	-3.058498	-4.475247	1.856743
C	-3.905108	-4.954398	2.868480
C	-4.484865	-6.229268	2.754992
C	-4.210418	-7.027129	1.630251
C	-3.358194	-6.553894	0.620086
N	4.328134	-0.512083	-3.441403
C	2.344321	-0.125831	-5.350315
C	2.605068	-0.642304	-6.636441
C	2.328077	0.131668	-7.775022
C	1.782494	1.419035	-7.639310
C	1.518396	1.936548	-6.359298
C	1.796302	1.168970	-5.219058
N	4.328368	0.511435	3.441649
C	2.344460	0.125600	5.350536
C	2.605230	0.642217	6.636601
C	2.328079	-0.131570	7.775270
C	1.782332	-1.418877	7.639702
C	1.518212	-1.936529	6.359753

C	1.796262	-1.169136	5.219420
C	6.523174	-0.409223	-1.851496
C	7.702029	0.359482	-1.817085
C	8.946677	-0.273476	-1.664443
C	9.024188	-1.668798	-1.537863
C	7.848483	-2.439703	-1.564142
C	6.604219	-1.814916	-1.720561
N	-0.055177	5.288232	-0.048515
C	-2.775498	5.272318	-0.725541
C	-3.357290	6.554256	-0.619641
C	-4.209398	7.027661	-1.629824
C	-4.483992	6.229850	-2.754563
C	-3.904522	4.954846	-2.868009
C	-3.058035	4.475532	-1.856248
C	2.678282	5.332198	-0.152490
C	3.286006	4.763587	0.987071
C	4.358687	5.418461	1.610901
C	4.827914	6.643824	1.106268
C	4.223489	7.214280	-0.027005
C	3.154393	6.559608	-0.659544
H	-0.001350	-6.316676	0.069226
H	-4.591955	0.852815	4.267763
H	-4.591325	-0.853665	-4.267559
H	-4.831303	-2.530014	0.229741
H	-4.830867	2.530021	-0.229534
H	-0.526556	-7.220316	4.706518
H	-0.607862	-6.358515	2.369108
H	2.695874	-7.001348	1.558282
H	-0.557559	-3.969842	-7.408873
H	-5.896923	-4.767005	0.522610
H	-7.726117	-0.823038	-1.246538
H	1.277210	-6.452690	6.275593
H	-4.808511	2.943430	-7.230308
H	2.920747	-3.801396	-1.380274
H	-4.575745	0.906073	-5.821618
H	-7.725835	0.822953	1.245468
H	0.144556	-6.341758	-2.266745
H	-6.408286	2.312231	3.821247
H	-9.590003	-0.828583	1.399239
H	-4.103049	-4.331098	3.753595
H	-2.613552	-3.470629	1.943053
H	4.818842	-4.971124	-2.504058
H	-9.590149	0.828596	-1.400965
H	-3.092489	4.768450	-7.106757
H	-0.930063	2.528533	-4.083774
H	-5.032895	2.066876	-3.068424
H	5.666710	-7.158183	-1.599473
H	-0.557436	3.969783	7.408791
H	-5.896127	4.767191	-0.522392
H	-0.403205	-7.643136	-4.324321
H	-9.187830	-3.102161	2.375326
H	-5.033556	-2.066851	3.068911
H	-7.413697	4.569837	3.545962

H	-6.408043	-2.312334	-3.821317
H	4.588976	-8.173231	0.424965
H	2.927418	-3.937133	3.152215
H	-3.150730	-7.184465	-0.258226
H	-7.413791	-4.569815	-3.546006
H	-7.185169	5.801032	1.373011
H	-6.897936	3.712212	-3.216083
H	2.993092	-4.791465	5.483768
H	-9.187417	3.102292	-2.376538
H	-0.927919	0.223823	-6.378038
H	-0.930259	-2.528654	4.083020
H	-4.661377	-8.027271	1.539966
H	-2.724597	-7.592593	-5.273930
H	-2.662472	-2.827658	-3.796039
H	-3.977062	-4.949409	-2.074388
H	-3.091440	-4.768930	7.106643
H	-1.832266	-4.593460	-5.332500
H	-4.807476	-2.943970	7.231034
H	-5.150204	-6.605180	3.547436
H	-6.898760	-3.712062	3.216021
H	-4.575288	-0.906455	5.822472
H	-4.500602	-6.213116	-4.146457
H	-7.185798	-5.800828	-1.372916
H	-1.151440	4.554155	-5.522036
H	-1.151028	-4.554440	5.521198
H	-0.110228	-1.550579	-7.911843
H	-0.928167	-0.223936	6.378263
H	-0.110144	1.550529	7.911848
H	-1.832342	4.593351	5.332553
H	-2.662893	2.827469	3.796306
H	-0.000691	6.316865	-0.068798
H	5.014229	0.533622	4.207718
H	5.014111	-0.534583	-4.207363
H	5.179530	2.750280	-0.496033
H	5.177643	-2.750134	0.495106
H	-0.403357	7.643565	4.324883
H	0.144797	6.342231	2.267352
H	-3.149716	7.184806	0.258659
H	1.558579	2.019484	-8.534212
H	5.770173	5.098655	-1.101870
H	7.652855	1.454531	-1.909730
H	-2.724840	7.592684	5.274248
H	5.278188	-5.052736	-5.484412
H	-2.613356	3.470793	-1.942494
H	5.126121	-2.717943	-4.631705
H	7.653102	-1.454556	1.909998
H	-0.608373	6.358294	-2.368510
H	5.150694	-1.673447	4.706943
H	9.864089	-0.334119	1.643371
H	4.820605	4.969941	2.502710
H	2.922054	3.800584	1.379357
H	-4.102577	4.331569	-3.753117
H	9.863832	0.334191	-1.642785

H	3.214109	-6.462150	-5.682908
H	0.819434	-3.171082	-4.176421
H	5.684343	-2.420997	-1.758117
H	-5.149229	6.605899	-3.547029
H	1.558293	-2.019170	8.534678
H	5.768769	-5.098695	1.099800
H	-0.527835	7.220124	-4.705907
H	10.002655	2.158717	1.419165
H	5.684449	2.420880	1.757970
H	5.729078	-4.019614	5.307099
H	5.148513	1.672561	-4.707582
H	-4.660153	8.027897	-1.539549
H	-3.976578	4.949215	2.074650
H	2.696140	7.001305	-1.558278
H	5.726755	4.018483	-5.308859
H	6.051682	-5.741865	3.511120
H	7.899768	-3.534897	-1.462810
H	-4.500512	6.212902	4.146651
H	10.002475	-2.158638	-1.418547
H	3.016551	-1.656893	-6.751261
H	0.819612	3.170502	4.176565
H	4.589849	8.172718	-0.425510
H	1.275795	6.453038	-6.275394
H	1.571315	1.565240	-4.215607
H	2.927348	3.937805	-3.152475
H	3.214381	6.462303	5.681298
H	1.082076	2.939712	-6.245016
H	5.278499	5.052935	5.482980
H	5.668322	7.157128	1.598257
H	7.899886	3.534882	1.463022
H	5.126411	2.717791	4.631141
H	2.992303	4.792246	-5.483982
H	6.051045	5.741183	-3.513603
H	0.982488	-5.507170	-5.019347
H	0.982671	5.506901	5.018633
H	2.536240	-0.276577	-8.776068
H	3.016841	1.656769	6.751298
H	2.536260	0.276780	8.776267
H	1.081749	-2.939641	6.245579
H	1.571214	-1.565487	4.216012
H	-2.397988	-1.588250	0.573356
H	2.564836	-1.625931	-0.529879
H	-0.129479	-2.025636	-2.128537
H	0.534602	1.109582	-2.209045
H	2.564295	1.625677	0.530480
H	-0.131116	2.022492	2.129756
H	0.534324	-1.110253	2.209292
H	-2.398460	1.588685	-0.573250

Table S15: Cartesian coordinates for **7b**$^{2+}$.

C	-6.043504	-3.024043	-2.816826
C	-5.555322	-2.305189	-1.703542
C	-5.612166	-2.893753	-0.423363
C	-6.170172	-4.170286	-0.252501
C	-6.664093	-4.874850	-1.361318
C	-6.594607	-4.302926	-2.644624
P	-4.896411	-0.593622	-1.827751
N	-4.182727	-0.507812	-3.393169
P	-2.609979	0.086227	-3.765487
C	-2.886601	1.557056	-4.838887
C	-4.130890	1.851221	-5.433903
C	-4.271696	2.984836	-6.250287
C	-3.174165	3.832631	-6.479020
C	-1.937416	3.553025	-5.875408
C	-1.794223	2.426429	-5.051305
Ag	-3.395078	0.115628	0.022588
P	-4.847859	0.796060	1.922885
N	-4.066333	0.808376	3.460672
P	-2.504472	0.163485	3.816964
C	-2.791541	-1.243940	4.973853
C	-1.959940	-2.377106	4.862672
C	-2.148673	-3.479734	5.711620
C	-3.175381	-3.463295	6.667972
C	-4.012181	-2.338262	6.781684
C	-3.818325	-1.231132	5.943076
Ag	-1.274373	-0.580015	1.803294
Ag	1.198346	0.872529	1.811531
P	2.667975	0.795803	3.799429
C	3.112523	2.464685	4.442609
C	2.094524	3.442800	4.451917
C	2.348487	4.721360	4.971300
C	3.621433	5.040007	5.472801
C	4.644520	4.076163	5.448219
C	4.392711	2.792678	4.936252
Ag	-1.180759	2.228428	0.682909
Ag	-1.252502	0.699620	-1.786469
Ag	1.115126	-0.924274	-1.841845
P	2.571397	-0.990740	-3.844116
C	2.820694	-2.687987	-4.515298
C	4.031349	-3.128252	-5.091555
C	4.130420	-4.424840	-5.621431
C	3.021708	-5.288924	-5.584820
C	1.817915	-4.858179	-5.003985
C	1.718324	-3.567178	-4.463112
P	-1.316815	4.720263	0.194370
C	-1.431689	5.823793	1.660291
C	-0.274292	6.411857	2.214452
C	-0.373656	7.220277	3.358903
C	-1.620316	7.442213	3.966266
C	-2.771119	6.832177	3.435899
C	-2.679291	6.020425	2.295795

N	0.128257	5.270012	-0.564879
P	1.482391	4.354876	-1.119368
C	1.694358	4.958210	-2.842825
C	0.646776	5.596020	-3.538493
C	0.845152	6.035006	-4.858645
C	2.079508	5.830078	-5.496556
C	3.114277	5.163525	-4.815837
C	2.923845	4.722922	-3.499013
C	2.863910	5.169705	-0.204528
C	3.451669	6.381446	-0.627074
C	4.424536	7.006672	0.168690
C	4.816505	6.428507	1.388669
C	4.232168	5.223465	1.815081
C	3.259852	4.594342	1.021897
Ag	1.346920	1.871935	-0.908886
Ag	3.340742	-0.105238	-0.025295
P	4.815106	0.131579	-2.024941
N	4.153648	-0.378262	-3.533541
C	-2.606764	5.359002	-0.964007
C	-3.112117	6.676648	-0.926901
C	-4.033004	7.104727	-1.896972
C	-4.451710	6.226316	-2.911855
C	-3.942465	4.917451	-2.961897
C	-3.025926	4.485075	-1.991149
Ag	1.225809	-1.939251	0.869374
P	1.188522	-4.417057	1.066396
N	-0.233451	-5.240842	0.541370
P	-1.652586	-4.579488	-0.181235
C	-1.872808	-5.627265	-1.672837
C	-0.798735	-6.346210	-2.237807
C	-0.997609	-7.105555	-3.403401
C	-2.258982	-7.144911	-4.019864
C	-3.323492	-6.404381	-3.475204
C	-3.132447	-5.643546	-2.313455
Ag	-1.348831	-2.098387	-0.660780
C	-1.844274	1.491352	4.898391
C	-1.203653	1.212201	6.122295
C	-0.700310	2.264149	6.904578
C	-0.819284	3.592248	6.468956
C	-1.437990	3.872870	5.238413
C	-1.946195	2.829470	4.453643
P	4.814529	-0.474876	1.963632
C	6.390754	0.483291	1.938670
C	7.660283	-0.108655	1.790209
C	8.809262	0.698600	1.733213
C	8.702103	2.095372	1.817042
C	7.436282	2.690896	1.962469
C	6.288342	1.890793	2.021143
C	-6.401188	0.450099	-2.022016
C	-7.718231	-0.049814	-1.980744
C	-8.806695	0.833128	-2.082601
C	-8.589760	2.213336	-2.223469
C	-7.276930	2.715947	-2.267137

C	-6.188940	1.840141	-2.163275
N	4.162547	-0.008723	3.493385
C	5.378263	-2.207117	2.228249
C	5.332554	-3.087775	1.129601
C	5.796395	-4.406954	1.254953
C	6.290984	-4.862005	2.486358
C	6.328503	-3.993281	3.592365
C	5.879640	-2.670525	3.464445
C	2.137386	-0.106448	5.315222
C	2.173419	0.459798	6.605549
C	1.766949	-0.295670	7.718038
C	1.318211	-1.615169	7.551691
C	1.285471	-2.185374	6.267134
C	1.689438	-1.436946	5.153425
C	6.343692	-0.895313	-1.947181
C	7.594371	-0.368863	-1.567567
C	8.703141	-1.221443	-1.435929
C	8.573623	-2.599069	-1.671251
C	7.325790	-3.128917	-2.044013
C	6.216674	-2.283857	-2.180275
C	5.468212	1.823185	-2.350381
C	5.486133	2.735343	-1.277487
C	6.045455	4.013261	-1.437396
C	6.566326	4.398452	-2.682054
C	6.529741	3.502191	-3.766064
C	5.989681	2.218171	-3.601238
C	-2.036349	-1.220934	-4.925066
C	-1.480667	-0.936567	-6.187539
C	-1.064781	-1.986955	-7.022131
C	-1.187118	-3.319422	-6.601766
C	-1.725956	-3.606139	-5.335507
C	-2.145398	-2.564725	-4.497975
C	2.128647	-0.006312	-5.336266
C	1.987427	-0.569871	-6.620036
C	1.657298	0.245996	-7.715135
C	1.459266	1.623344	-7.536449
C	1.600907	2.190066	-6.257176
C	1.930748	1.382350	-5.160847
C	2.495526	-5.326219	0.134605
C	3.012746	-6.568350	0.559898
C	3.921991	-7.265180	-0.251577
C	4.320583	-6.727640	-1.488043
C	3.810120	-5.489054	-1.913936
C	2.902438	-4.788079	-1.104885
C	1.397074	-5.008832	2.793547
C	0.357090	-5.649979	3.497041
C	0.559222	-6.063807	4.825141
C	1.787490	-5.826532	5.463344
C	2.815769	-5.161533	4.772056
C	2.623903	-4.751034	3.446012
C	-2.962913	-5.169117	0.979495
C	-3.282437	-4.321024	2.061909
C	-4.187295	-4.741130	3.048370

C	-4.792837	-6.005636	2.953905
C	-4.485001	-6.851713	1.874241
C	-3.570726	-6.439640	0.891736
C	-6.287419	-0.322825	2.163248
C	-7.477918	-0.132854	1.429181
C	-8.504509	-1.086943	1.495828
C	-8.356097	-2.234993	2.291285
C	-7.174719	-2.424940	3.027242
C	-6.142104	-1.477333	2.962266
C	-5.616214	2.462598	1.816162
C	-5.180123	3.345297	0.808745
C	-5.761027	4.617712	0.681092
C	-6.765893	5.021631	1.574038
C	-7.198411	4.149941	2.589741
C	-6.635276	2.871018	2.705480
H	-0.221979	-6.264708	0.654058
H	-4.578769	1.254908	4.232877
H	-4.757774	-0.809102	-4.190366
H	-5.215608	-2.352489	0.449314
H	-4.388229	3.027318	0.112759
H	-0.248019	-6.588218	5.359941
H	-0.612589	-5.828128	3.006630
H	2.710072	-6.990722	1.530902
H	-0.859498	-4.138408	-7.259808
H	-6.200996	-4.616042	0.752491
H	-7.895790	-1.128658	-1.858201
H	1.943906	-6.157015	6.501340
H	-5.246344	3.205910	-6.711587
H	2.508438	-3.812195	-1.432062
H	-5.002776	1.204588	-5.252616
H	-7.606992	0.762175	0.802166
H	0.196095	-6.315839	-1.766824
H	-7.008175	2.179130	3.477976
H	-9.429323	-0.927999	0.920424
H	-4.411186	-4.078325	3.897375
H	-2.819135	-3.323480	2.128475
H	4.110968	-5.067216	-2.884549
H	-9.833424	0.437254	-2.051595
H	-3.287998	4.718783	-7.121651
H	-0.825141	2.219422	-4.569200
H	-5.162273	2.239701	-2.183149
H	5.031485	-7.278067	-2.123324
H	-0.424570	4.412624	7.087201
H	-5.425229	5.289901	-0.122524
H	-0.158446	-7.679936	-3.825408
H	-9.164263	-2.980135	2.340897
H	-5.217533	-1.631602	3.539463
H	-7.990893	4.463753	3.286037
H	-6.004630	-2.591595	-3.828883
H	4.322130	-8.234201	0.083971
H	3.438304	-4.236258	2.912773
H	-3.333230	-7.109803	0.051391
H	-6.975957	-4.854929	-3.517298

H	-7.223058	6.018027	1.474792
H	-7.096350	3.797014	-2.370112
H	3.778071	-4.958620	5.265605
H	-9.446136	2.900502	-2.297891
H	-1.375381	0.104051	-6.529544
H	-1.159425	-2.394668	4.104256
H	-4.955762	-7.843970	1.799572
H	-2.412930	-7.748971	-4.926735
H	-2.568793	-2.802069	-3.509022
H	-3.975923	-5.073497	-1.894746
H	-3.328527	-4.330272	7.328549
H	-1.821184	-4.646183	-4.991156
H	-4.817096	-2.322169	7.532213
H	-5.505298	-6.335568	3.725565
H	-7.053317	-3.319199	3.657355
H	-4.476819	-0.354378	6.045666
H	-4.313189	-6.417238	-3.956773
H	-7.095583	-5.878574	-1.229035
H	-1.076142	4.219161	-6.033334
H	-1.492893	-4.357028	5.611251
H	-0.645209	-1.755169	-8.012191
H	-1.098815	0.173882	6.472138
H	-0.214322	2.037632	7.864959
H	-1.526650	4.909149	4.882478
H	-2.434302	3.059883	3.493065
H	0.202356	6.289068	-0.696261
H	4.773315	-0.149926	4.308240
H	4.782304	-0.310930	-4.344406
H	5.051193	2.441724	-0.310972
H	4.922128	-2.739466	0.170033
H	0.533496	7.688769	3.770953
H	0.709231	6.241349	1.749797
H	-2.792595	7.370185	-0.133816
H	1.198458	2.259920	-8.395623
H	6.052624	4.712307	-0.588260
H	7.706119	0.707824	-1.369195
H	-1.696398	8.085728	4.855691
H	5.078097	-4.760334	-6.069714
H	-2.628787	3.457316	-2.028757
H	4.907696	-2.463015	-5.127557
H	7.755302	-1.202034	1.715315
H	-0.324908	5.756670	-3.046336
H	5.928471	-2.003961	4.339887
H	9.797982	0.227221	1.623642
H	4.526392	4.772255	2.774296
H	2.805782	3.646395	1.353455
H	-4.252818	4.229303	-3.762238
H	9.677525	-0.800319	-1.145035
H	3.101941	-6.303476	-6.003936
H	0.777346	-3.236075	-3.994689
H	5.240969	-2.704504	-2.470056
H	-5.172595	6.566099	-3.671201
H	0.996665	-2.203404	8.424597

H	5.749298	-5.081815	0.387971
H	0.029409	6.553352	-5.385988
H	9.605516	2.722127	1.771237
H	5.299743	2.363138	2.135508
H	6.716882	-4.347390	4.559619
H	5.983264	1.527928	-4.459364
H	-4.424329	8.132975	-1.861051
H	-3.588757	5.548455	1.892663
H	3.154842	6.836422	-1.584783
H	6.934272	3.802746	-4.744749
H	6.643569	-5.899345	2.590103
H	7.212656	-4.208695	-2.227328
H	-3.750660	6.989021	3.912590
H	9.446089	-3.261505	-1.566410
H	2.133129	-1.649931	-6.767877
H	1.096670	3.202019	4.050426
H	4.879509	7.951368	-0.166313
H	2.235544	6.185467	-6.526419
H	2.035895	1.834407	-4.161159
H	3.743930	4.210021	-2.973465
H	3.821947	6.044270	5.876059
H	1.459334	3.270348	-6.108667
H	5.646180	4.323013	5.832150
H	5.578463	6.921670	2.011728
H	7.339926	3.785901	2.026696
H	5.204911	2.049888	4.917083
H	4.080703	4.983318	-5.310419
H	6.995437	5.403303	-2.813653
H	0.947329	-5.529587	-4.958499
H	1.543683	5.472098	4.972838
H	1.557802	-0.200824	-8.716432
H	2.514334	1.496346	6.744477
H	1.803930	0.152408	8.723063
H	0.946621	-3.221976	6.128107
H	1.656078	-1.888871	4.149211
H	-0.231597	-2.142936	-2.028301
H	-2.404974	1.647406	-0.563784
H	-0.023835	2.205960	2.022535
H	-2.498249	-1.475773	0.630305
H	0.461455	1.053275	-2.280356
H	2.449206	-1.699790	-0.506193
H	2.568053	1.549863	0.444810
H	0.432370	-1.040021	2.241573

Table S16: Cartesian coordinates for $[Ag_{10}(dppa)_6]^{2+}$ via $\mathbf{7a}^{2+}$.

C	4.851668	3.891316	-1.157965
C	4.689748	4.482590	0.113649
C	4.654282	5.878095	0.244315
C	4.768968	6.694239	-0.892945
C	4.920714	6.110840	-2.162266
C	4.957864	4.713770	-2.298634
P	4.906247	2.059532	-1.228659
C	6.672406	1.630036	-0.945979
C	7.631731	2.552699	-0.482828
C	8.931820	2.118138	-0.174783
C	9.283076	0.766756	-0.321994
C	8.328775	-0.157163	-0.784419
C	7.030092	0.268597	-1.092602
Ag	3.613543	0.724845	0.349614
P	4.439705	0.710635	2.637113
C	5.587919	-0.687238	2.983509
C	5.990826	-1.520414	1.920253
C	6.834013	-2.618027	2.157574
C	7.269231	-2.896227	3.462252
C	6.879176	-2.065094	4.528050
C	6.050037	-0.958662	4.290024
Ag	1.784013	0.266028	-1.640707
P	3.408686	0.580522	-3.453208
C	4.284362	-0.974487	-3.905969
C	3.523852	-2.160468	-3.951669
C	4.129829	-3.374511	-4.308084
C	5.505072	-3.419705	-4.593258
C	6.273388	-2.244877	-4.525532
C	5.665303	-1.024761	-4.188417
Ag	0.908131	-0.002446	1.001462
P	1.462299	0.342420	3.352468
C	0.688600	1.852873	4.085204
C	1.311375	2.626185	5.088122
C	0.660745	3.749485	5.625583
C	-0.612079	4.115868	5.159882
C	-1.235294	3.351798	4.161166
C	-0.589302	2.230029	3.625731
Ag	2.736486	-1.885683	0.128564
P	2.908645	-4.233011	0.895645
C	2.817191	-4.611405	2.687721
C	2.083831	-5.702382	3.196550
C	2.082853	-5.965054	4.575967
C	2.802234	-5.137927	5.453880
C	3.513316	-4.035618	4.951796
C	3.517074	-3.766416	3.576721
Ag	0.355067	2.427295	-0.309079
P	-0.046994	4.887643	-0.102799
C	0.130989	5.754227	-1.713745
C	-0.904046	6.509524	-2.301090
C	-0.697491	7.145361	-3.537369
C	0.534703	7.019944	-4.199877

C	1.561997	6.248881	-3.626122
C	1.363204	5.615426	-2.391090
N	-1.636697	5.290635	0.440554
P	-2.981306	4.208820	0.555126
C	-3.881413	4.833372	2.022988
C	-3.347104	5.801989	2.898798
C	-4.071179	6.199492	4.034867
C	-5.327405	5.634603	4.307982
C	-5.855941	4.658309	3.445121
C	-5.136759	4.251753	2.313001
C	0.983719	5.898666	1.036104
C	1.334525	7.237068	0.757985
C	2.041162	7.989743	1.708472
C	2.402455	7.412293	2.937619
C	2.065938	6.075659	3.210795
C	1.366607	5.314099	2.262769
Ag	-2.456172	1.811908	0.338032
Ag	-1.726331	-0.775046	1.466212
P	-3.354555	-0.970566	3.294379
C	-3.390827	-2.623314	4.110181
C	-3.926928	-2.836284	5.398496
C	-3.958626	-4.129836	5.941689
C	-3.464100	-5.219079	5.203399
C	-2.937725	-5.014715	3.917068
C	-2.897428	-3.721297	3.374376
Ag	-3.645429	-0.553294	-0.536391
P	-4.073510	-1.579493	-2.694008
C	-4.355314	-3.386605	-2.874928
C	-5.277171	-4.010577	-2.003942
C	-5.545511	-5.382250	-2.122617
C	-4.879090	-6.152747	-3.089632
C	-3.941067	-5.542624	-3.937542
C	-3.676041	-4.167636	-3.832719
Ag	-0.951717	0.018486	-1.141645
P	-1.378228	-0.323316	-3.511666
C	-1.621555	1.261743	-4.427610
C	-1.035655	2.440371	-3.927444
C	-1.192235	3.656915	-4.607443
C	-1.941528	3.709990	-5.792806
C	-2.540537	2.541588	-6.294862
C	-2.383073	1.323998	-5.615729
Ag	-0.098681	-2.474715	-0.124058
P	0.384141	-4.910092	-0.691050
C	0.615188	-5.834652	-2.273943
C	1.913860	-6.043300	-2.789220
C	2.094832	-6.758352	-3.984007
C	0.985825	-7.258733	-4.685935
C	-0.309320	-7.032489	-4.188244
C	-0.498464	-6.326156	-2.991104
P	-5.490462	-0.689061	1.084670
C	-6.561566	0.802292	0.950633
C	-6.469038	1.572204	-0.227572
C	-7.290284	2.696562	-0.409560

C	-8.201140	3.065441	0.593181
C	-8.293761	2.306291	1.774273
C	-7.480251	1.176596	1.953674
N	-4.985346	-0.788479	2.727339
C	-3.301384	0.218389	4.687288
C	-2.342243	0.043765	5.708663
C	-2.242672	0.979731	6.746508
C	-3.091972	2.098556	6.772908
C	-4.035762	2.283721	5.750096
C	-4.139636	1.352608	4.704606
N	-2.848180	-1.208764	-3.827393
C	-0.291377	-1.299282	-4.643031
C	0.359875	-0.742144	-5.762247
C	1.089041	-1.568885	-6.634384
C	1.176519	-2.948544	-6.399075
C	0.553650	-3.505242	-5.267798
C	-0.164824	-2.685304	-4.388072
C	-6.683034	-2.079652	0.953104
C	-7.782925	-1.997438	0.068152
C	-8.585236	-3.124360	-0.165635
C	-8.306005	-4.342583	0.478167
C	-7.215943	-4.427987	1.361622
C	-6.403881	-3.307630	1.596533
C	-5.581981	-0.783123	-3.392241
C	-6.828283	-1.430323	-3.518248
C	-7.962016	-0.703320	-3.916703
C	-7.865605	0.669793	-4.193278
C	-6.623607	1.317383	-4.077830
C	-5.488064	0.599760	-3.677151
C	-4.068825	4.672248	-0.860732
C	-3.840720	4.006384	-2.085073
C	-4.572910	4.359295	-3.228474
C	-5.551784	5.364915	-3.152994
C	-5.790321	6.023744	-1.933967
C	-5.050031	5.683502	-0.790411
N	3.146719	0.520387	3.758746
C	0.973261	-0.962014	4.568929
C	1.106080	-0.751699	5.959663
C	0.717591	-1.749459	6.867105
C	0.180704	-2.958911	6.393649
C	0.055163	-3.175476	5.013274
C	0.453875	-2.185050	4.102236
N	4.649807	1.648005	-2.880093
C	3.056507	1.402001	-5.061890
C	3.457143	0.885884	-6.310723
C	3.117095	1.565076	-7.492885
C	2.380703	2.759319	-7.437529
C	1.983414	3.279890	-6.192588
C	2.314048	2.603462	-5.011529
C	5.377399	2.176991	3.218689
C	6.771736	2.243238	2.995335
C	7.468864	3.436960	3.232515
C	6.790447	4.576567	3.695214

C	5.404072	4.516665	3.916451
C	4.697495	3.329317	3.673448
N	1.829169	-5.356157	0.137559
C	-0.990364	-5.877295	0.069718
C	-0.810562	-7.171721	0.600158
C	-1.907637	-7.886833	1.102950
C	-3.194111	-7.318850	1.070814
C	-3.379886	-6.030514	0.546181
C	-2.281067	-5.308041	0.051895
C	4.560485	-4.873960	0.394474
C	5.129734	-4.343466	-0.785726
C	6.395568	-4.770832	-1.212569
C	7.105754	-5.723442	-0.460431
C	6.545528	-6.250657	0.715778
C	5.277281	-5.827891	1.146210
H	-1.847926	6.296848	0.502608
H	-3.018824	-1.470332	-4.807179
H	-5.714511	-1.002155	3.421382
H	-5.746275	1.291343	-1.010832
H	-5.791319	-3.424993	-1.226213
H	-1.509900	7.736531	-3.986478
H	-1.882330	6.592021	-1.803562
H	1.056957	7.691590	-0.205537
H	-3.011597	2.832860	7.588576
H	-7.203357	3.288403	-1.333071
H	-8.009664	-1.050855	-0.447078
H	0.693795	7.518555	-5.168023
H	-4.372978	-4.288734	6.949038
H	1.104819	4.266167	2.481505
H	-4.308017	-1.986409	5.986020
H	-6.920962	-2.506262	-3.308451
H	-2.352037	6.232338	2.708827
H	-2.929766	-3.709196	-4.498628
H	-8.929052	-1.219559	-4.017543
H	-4.366201	3.848859	-4.181424
H	-3.079925	3.209992	-2.147474
H	2.339557	5.618966	4.173278
H	-9.440826	-3.047810	-0.853900
H	-3.488022	-6.231354	5.635308
H	-2.460223	-3.555444	2.374919
H	-5.546532	-3.389571	2.283094
H	2.950194	8.007045	3.684719
H	1.739859	-3.593047	-7.090543
H	-6.279315	-5.847444	-1.447167
H	-3.649340	6.960664	4.708933
H	-8.757507	1.234742	-4.503498
H	-4.518007	1.114027	-3.581558
H	-3.413588	-6.138137	-4.698405
H	-7.574006	0.582999	2.876865
H	2.308289	9.034815	1.489146
H	2.178802	5.022731	-1.945328
H	-5.241150	6.202568	0.161574
H	-9.013519	2.591375	2.556997

H	-5.087643	-7.229455	-3.179141
H	-6.996354	-5.374517	1.879824
H	2.527139	6.136513	-4.142620
H	-8.943040	-5.221527	0.297525
H	-1.676442	-0.831472	5.698416
H	-0.455060	2.396017	-2.989311
H	-6.555988	6.812295	-1.873897
H	-5.895020	5.954561	5.194962
H	-4.871631	1.506516	3.896744
H	-5.559680	3.484761	1.645776
H	-2.063917	4.666229	-6.324360
H	-4.690614	3.167888	5.752952
H	-3.133027	2.576259	-7.221904
H	-6.130249	5.640220	-4.048346
H	-6.537764	2.393220	-4.293660
H	-2.860467	0.419793	-6.022982
H	-6.836943	4.204237	3.651387
H	-8.841810	3.950036	0.458074
H	-2.546760	-5.860667	3.332783
H	-0.732057	4.567599	-4.203195
H	-1.492001	0.831943	7.537634
H	0.290862	0.336742	-5.965538
H	1.583990	-1.121966	-7.509114
H	0.628316	-4.582905	-5.066108
H	-0.645750	-3.129313	-3.502060
H	2.143545	-6.333658	0.068022
H	5.328591	1.984466	-3.574486
H	3.394646	0.303567	4.732384
H	5.622649	-1.314244	0.902212
H	4.592970	3.849369	1.010285
H	3.113407	-6.933433	-4.363624
H	2.790786	-5.658908	-2.246061
H	0.187576	-7.637939	0.609258
H	-0.142879	-3.735368	7.103312
H	7.135833	-3.265716	1.320554
H	7.315193	1.361878	2.621075
H	1.129557	-7.826595	-5.617267
H	1.154821	4.341534	6.411559
H	-2.430982	-4.292049	-0.352162
H	2.315647	2.357426	5.449500
H	7.363814	3.612211	-0.354488
H	1.507503	-6.345611	2.514337
H	5.056601	4.267166	-3.300063
H	9.676922	2.845819	0.181856
H	6.827064	-4.348417	-2.132836
H	4.585624	-3.577120	-1.365284
H	-4.379862	-5.573451	0.529249
H	8.554207	3.473923	3.053085
H	-1.122860	4.998464	5.574125
H	-1.082527	1.641576	2.832637
H	3.607941	3.298446	3.823575
H	-4.053504	-7.883988	1.462799
H	2.114060	3.285772	-8.366433

H	4.519233	6.324886	1.240260
H	1.513500	-6.822330	4.966820
H	10.302395	0.431699	-0.077491
H	6.282270	-0.460763	-1.445666
H	5.009661	6.749164	-3.054683
H	5.775039	-0.296775	5.127794
H	-1.760545	-8.897771	1.512670
H	-1.518704	-6.175669	-2.605697
H	4.849194	-6.229116	2.078026
H	7.231057	-2.276445	5.549323
H	4.730851	7.789341	-0.790965
H	4.864777	5.407214	4.273543
H	-1.182845	-7.425143	-4.731098
H	7.341232	5.510490	3.882547
H	1.476018	0.210043	6.349134
H	2.447646	-2.132930	-3.715740
H	7.102281	-6.994421	1.305964
H	2.796879	-5.345049	6.534581
H	0.341593	-2.349640	3.017275
H	4.070636	-2.895913	3.193830
H	5.980068	-4.373442	-4.870291
H	-0.358284	-4.121584	4.638835
H	7.351580	-2.274521	-4.745889
H	8.102754	-6.053753	-0.789764
H	8.595420	-1.219280	-0.898961
H	6.277224	-0.111329	-4.139841
H	4.062544	-3.369638	5.634040
H	7.917808	-3.764820	3.652437
H	-2.234458	3.626095	3.799466
H	3.518159	-4.286774	-4.361008
H	0.815103	-1.572127	7.949166
H	4.029986	-0.052158	-6.360850
H	3.433815	1.157749	-8.465455
H	1.397378	4.209771	-6.139458
H	1.984685	3.002770	-4.038386

Table S17: Cartesian coordinates for **$[Ag_{10}(dppa)_6]^{2+}$** via **$7b^{2+}$**.

C	-3.675914	-4.168004	-3.832049
C	-4.355640	-3.386951	-2.874576
C	-5.277846	-4.010952	-2.004017
C	-5.546129	-5.382633	-2.122821
C	-4.879321	-6.153114	-3.089564
C	-3.940899	-5.542980	-3.937015
P	-4.073677	-1.579840	-2.693769
N	-2.848213	-1.209530	-3.827116
P	-1.378425	-0.323684	-3.511488
C	-1.622301	1.261307	-4.427438
C	-2.383556	1.323268	-5.615737
C	-2.541461	2.540819	-6.294830
C	-1.943166	3.709489	-5.792542
C	-1.194141	3.656708	-4.606995

C	-1.037112	2.440191	-3.927047
Ag	-3.645378	-0.553253	-0.536447
P	-5.490167	-0.689534	1.085235
N	-4.984901	-0.789084	2.727854
P	-3.354004	-0.970876	3.294624
C	-3.389453	-2.623816	4.110007
C	-2.895655	-3.721390	3.373892
C	-2.935112	-5.014940	3.916336
C	-3.461095	-5.219823	5.202739
C	-3.956088	-4.130987	5.941336
C	-3.925206	-2.837316	5.398393
Ag	-1.726092	-0.774184	1.466480
Ag	0.908542	-0.002412	1.001226
P	1.463157	0.342694	3.352140
C	0.689345	1.853238	4.084694
C	-0.588829	2.229975	3.625667
C	-1.234890	3.351679	4.161161
C	-0.611474	4.116110	5.159479
C	0.661631	3.750147	5.624725
C	1.312319	2.626897	5.087217
Ag	-2.456628	1.811915	0.338364
Ag	-0.951772	0.018564	-1.141487
Ag	1.784003	0.266001	-1.641145
P	3.408123	0.580909	-3.453939
C	4.284211	-0.973766	-3.907018
C	5.664982	-1.023517	-4.190408
C	6.273399	-2.243500	-4.527403
C	5.505609	-3.418741	-4.594018
C	4.130544	-3.374072	-4.307943
C	3.524243	-2.160131	-3.951700
P	-2.981537	4.208828	0.555639
C	-3.881429	4.833217	2.023715
C	-3.347039	5.801735	2.899586
C	-4.071062	6.199207	4.035700
C	-5.327315	5.634381	4.308818
C	-5.855923	4.658162	3.445911
C	-5.136792	4.251648	2.313749
N	-1.636818	5.290453	0.441158
P	-0.047320	4.887416	-0.102812
C	0.130064	5.754006	-1.713794
C	-0.905103	6.509433	-2.300722
C	-0.698922	7.145292	-3.537060
C	0.533015	7.019761	-4.200014
C	1.560441	6.248572	-3.626658
C	1.362030	5.615095	-2.391584
C	0.983841	5.898387	1.035700
C	1.334408	7.236824	0.757425
C	2.041522	7.989526	1.707534
C	2.403522	7.412063	2.936463
C	2.067244	6.075398	3.209777
C	1.367435	5.313806	2.262131
Ag	0.355149	2.426960	-0.308888
Ag	3.613395	0.724926	0.349497

P	4.905616	2.059925	-1.229379
N	4.649004	1.648675	-2.880853
C	-4.069231	4.672554	-0.859968
C	-5.050156	5.684065	-0.789412
C	-5.790629	6.024520	-1.932784
C	-5.552539	5.365651	-3.151880
C	-4.573948	4.359772	-3.227596
C	-3.841593	4.006643	-2.084364
Ag	2.736354	-1.885815	0.128204
P	2.908399	-4.232865	0.895603
N	1.828758	-5.356260	0.138147
P	0.383853	-4.910071	-0.690631
C	0.615025	-5.834671	-2.273523
C	1.913768	-6.043056	-2.788757
C	2.094922	-6.758123	-3.983505
C	0.986035	-7.258773	-4.685441
C	-0.309169	-7.032777	-4.187795
C	-0.498489	-6.326440	-2.990682
Ag	-0.098997	-2.474761	-0.123318
C	-3.300818	0.217929	4.687656
C	-2.341568	0.043457	5.708949
C	-2.241986	0.979500	6.746728
C	-3.091342	2.098276	6.773131
C	-4.035231	2.283309	5.750384
C	-4.139149	1.352102	4.704986
P	4.440451	0.710995	2.636562
C	5.378396	2.177185	3.218155
C	6.772783	2.243111	2.995004
C	7.470144	3.436682	3.232257
C	6.791922	4.576461	3.694819
C	5.405495	4.516892	3.915819
C	4.698694	3.329697	3.672739
C	-5.582024	-0.783295	-3.391937
C	-6.828295	-1.430495	-3.518332
C	-7.961978	-0.703389	-3.916736
C	-7.865546	0.669802	-4.192907
C	-6.623575	1.317382	-4.077120
C	-5.488079	0.599669	-3.676471
N	3.147559	0.520897	3.758306
C	5.588541	-0.687030	2.982773
C	5.991169	-1.520251	1.919471
C	6.834330	-2.617929	2.156655
C	7.269772	-2.896125	3.461245
C	6.879940	-2.064961	4.527114
C	6.050840	-0.958484	4.289225
C	0.974210	-0.961380	4.569061
C	1.107528	-0.750743	5.959696
C	0.719204	-1.748208	6.867521
C	0.182036	-2.957719	6.394534
C	0.055978	-3.174596	5.014258
C	0.454444	-2.184426	4.102825
C	6.671628	1.629715	-0.946873
C	7.631253	2.551774	-0.483142

C	8.931157	2.116571	-0.175235
C	9.281938	0.765146	-0.323191
C	8.327346	-0.158159	-0.786231
C	7.028831	0.268232	-1.094263
C	4.851515	3.891703	-1.158609
C	4.690778	4.483130	0.113096
C	4.655375	5.878646	0.243608
C	4.768994	6.694672	-0.893841
C	4.919622	6.111124	-2.163216
C	4.956647	4.714037	-2.299457
C	-0.291477	-1.299474	-4.642913
C	0.359398	-0.742359	-5.762356
C	1.088590	-1.569068	-6.634502
C	1.176483	-2.948661	-6.398963
C	0.553995	-3.505320	-5.267459
C	-0.164522	-2.685419	-4.387737
C	3.055203	1.402359	-5.062433
C	3.455652	0.886376	-6.311393
C	3.114862	1.565319	-7.493483
C	2.377917	2.759209	-7.437953
C	1.980849	3.279668	-6.192897
C	2.312221	2.603482	-5.011905
C	4.560164	-4.874009	0.394406
C	5.276887	-5.828126	1.145967
C	6.545043	-6.250986	0.715366
C	7.105281	-5.723643	-0.460784
C	6.395202	-4.770795	-1.212714
C	5.129424	-4.343393	-0.785730
C	2.817219	-4.610647	2.687839
C	2.083735	-5.701390	3.197023
C	2.082978	-5.963835	4.576480
C	2.802680	-5.136682	5.454105
C	3.513846	-4.034589	4.951675
C	3.517428	-3.765644	3.576550
C	-0.990783	-5.877237	0.069961
C	-2.281478	-5.307987	0.051947
C	-3.380375	-6.030484	0.546004
C	-3.194704	-7.318864	1.070550
C	-1.908255	-7.886874	1.102838
C	-0.811090	-7.171725	0.600294
C	-6.682726	-2.080147	0.953731
C	-7.782710	-1.997942	0.068891
C	-8.585055	-3.124860	-0.164781
C	-8.305757	-4.343071	0.479016
C	-7.215613	-4.428462	1.362365
C	-6.403534	-3.308098	1.597188
C	-6.561406	0.801763	0.951476
C	-6.469063	1.571848	-0.226630
C	-7.290403	2.696180	-0.408347
C	-8.201165	3.064856	0.594556
C	-8.293605	2.305530	1.775551
C	-7.480004	1.175859	1.954677
H	2.142960	-6.333832	0.068901

H	-5.714021	-1.002488	3.422025
H	-3.019119	-1.470571	-4.806995
H	-5.792274	-3.425385	-1.226465
H	-5.746377	1.291137	-1.010016
H	1.513543	-6.820942	4.967584
H	1.507088	-6.344607	2.515060
H	4.848846	-6.229360	2.077802
H	1.739832	-3.593136	-7.090448
H	-6.280193	-5.847838	-1.447670
H	-6.920963	-2.506495	-3.308851
H	2.797522	-5.343613	6.534843
H	-3.133733	2.575270	-7.222019
H	4.585347	-3.576884	-1.365109
H	-2.860384	0.418852	-6.023188
H	-8.009474	-1.051366	-0.446339
H	2.790602	-5.658472	-2.245588
H	-7.573617	0.582098	2.877777
H	-9.440714	-3.048333	-0.852961
H	-4.380353	-5.573450	0.528951
H	-2.431306	-4.291970	-0.352076
H	6.826731	-4.348183	-2.132876
H	-8.928998	-1.219604	-4.017861
H	-2.065888	4.665693	-6.324084
H	-0.456711	2.396047	-2.988783
H	-4.518043	1.113925	-3.580571
H	8.102223	-6.054038	-0.790206
H	-3.010924	2.832651	7.588730
H	-7.203657	3.288181	-1.331773
H	3.113544	-6.933001	-4.363091
H	-8.942821	-5.222014	0.298468
H	-5.546145	-3.389989	2.283704
H	-9.013282	2.590458	2.558405
H	-2.929258	-3.709586	-4.497531
H	7.101739	-6.994931	1.305378
H	4.071158	-2.895345	3.193452
H	0.187055	-7.637917	0.609498
H	-3.413049	-6.138490	-4.697619
H	-8.841902	3.949432	0.459645
H	-6.537715	2.393280	-4.292636
H	4.063282	-3.368562	5.633706
H	-8.757413	1.234827	-4.503091
H	0.290044	0.336473	-5.965816
H	-2.458783	-3.555091	2.374364
H	-1.761244	-8.897843	1.512501
H	1.129904	-7.826649	-5.616742
H	-0.645184	-3.129425	-3.501583
H	-1.518763	-6.176143	-2.605301
H	-3.484366	-6.232186	5.634478
H	0.628982	-4.582927	-5.065599
H	-4.370153	-4.290318	6.948735
H	-4.054168	-7.884009	1.462366
H	-6.995978	-5.374988	1.880557
H	-4.306642	-1.987749	5.986137

H	-1.182593	-7.425634	-4.730667
H	-5.087871	-7.229811	-3.179215
H	-0.734500	4.567600	-4.202596
H	-2.543776	-5.860550	3.331803
H	1.583228	-1.122192	-7.509429
H	-1.675645	-0.831689	5.698677
H	-1.491263	0.831770	7.537815
H	-4.690124	3.167445	5.753217
H	-4.871254	1.505913	3.897205
H	-1.847698	6.296690	0.503997
H	3.395524	0.304660	4.732063
H	5.328004	1.984890	-3.575163
H	4.594801	3.850061	1.009919
H	5.622786	-1.314091	0.901503
H	-3.649153	6.960309	4.709801
H	-2.351933	6.232027	2.709686
H	-5.240916	6.203164	0.162629
H	2.110649	3.285466	-8.366787
H	4.521232	6.325545	1.239623
H	7.363709	3.611317	-0.354275
H	-5.894886	5.954307	5.195837
H	7.351451	-2.272728	-4.748494
H	-3.081044	3.210035	-2.146980
H	6.276563	-0.109810	-4.142679
H	7.316097	1.361630	2.620837
H	-1.883178	6.592050	-1.802799
H	5.775994	-0.296605	5.127051
H	8.555523	3.473409	3.052996
H	2.341437	5.618729	4.172105
H	1.105802	4.265862	2.481021
H	-4.367585	3.849304	-4.180606
H	9.676488	2.843778	0.181892
H	5.980901	-4.372375	-4.870900
H	2.448170	-2.132978	-3.715109
H	6.280787	-0.460662	-1.447813
H	-6.131138	5.641127	-4.047092
H	-0.141364	-3.733988	7.104486
H	7.135943	-3.265655	1.319593
H	-1.511418	7.736588	-3.985843
H	7.342907	5.510250	3.882222
H	3.609095	3.299094	3.822616
H	7.231969	-2.276357	5.548324
H	5.054408	4.267306	-3.300920
H	-6.556081	6.813263	-1.872518
H	-5.559770	3.484721	1.646485
H	1.056291	7.691359	-0.205933
H	5.007783	6.749345	-3.055781
H	7.918342	-3.764744	3.651331
H	8.593619	-1.220305	-0.901385
H	-6.836944	4.204134	3.652183
H	10.301119	0.429582	-0.078808
H	4.028913	-0.051397	-6.361681
H	-1.082259	1.641280	2.832876

H	2.308457	9.034622	1.488082
H	0.691818	7.518394	-5.168196
H	1.982955	3.002731	-4.038707
H	2.177726	5.022323	-1.946102
H	-1.122326	4.998648	5.573756
H	1.394384	4.209261	-6.139584
H	1.155882	4.342466	6.410388
H	2.951642	8.006820	3.683280
H	4.866349	5.407585	4.272780
H	2.316785	2.358443	5.448276
H	2.525371	6.136146	-4.143535
H	4.730938	7.789783	-0.791945
H	3.519235	-4.286628	-4.360026
H	-2.234283	3.625623	3.799828
H	3.431438	1.158044	-8.466122
H	1.477750	0.211049	6.348774
H	0.817089	-1.570612	7.949504
H	-0.357616	-4.120795	4.640211
H	0.341624	-2.349213	3.017940

S.7. Gaussian Cartesian Coordinates for isomers of $[Ag_{10}H_8(dppa)_6]^{2+}$ and $[Ag_{10}H_8(dppm)_6]^{2+}$ used for the gas-phase CCS calculations (Table 1)

Table S18: Cartesian coordinates for $[Ag_{10}H_8(dppm)_6]^{2+}$ via $\mathbf{7a}^{2+}$.

C	4.85934	1.83448	-2.97954
C	4.92385	3.00022	-2.18469
C	5.01929	4.26521	-2.78174
C	5.00739	4.38307	-4.18188
C	4.90847	3.23177	-4.97937
C	4.84895	1.96069	-4.38412
P	4.90585	0.23136	-2.08266
C	6.71938	-0.09521	-1.91253
C	7.70967	0.69754	-2.52499
C	9.06615	0.36293	-2.37938
C	9.44264	-0.76184	-1.62951
C	8.45839	-1.55448	-1.01514
C	7.10489	-1.21887	-1.14946
Ag	3.50108	-0.00001	-0.00004
P	4.90623	-0.23123	2.08229
C	4.85973	-1.83449	2.97886
C	4.92422	-3.00003	2.18372
C	5.01980	-4.26516	2.78045
C	5.00805	-4.38336	4.18057
C	4.90910	-3.23225	4.97833
C	4.84944	-1.96102	4.38340
Ag	1.28382	-0.90764	-1.83893
P	2.76703	-1.41615	-3.76137
C	2.85864	-3.19477	-4.24930
C	1.74927	-4.01282	-3.95091
C	1.77560	-5.38306	-4.25257
C	2.91271	-5.95721	-4.84129
C	4.02557	-5.15282	-5.13552
C	3.99986	-3.78010	-4.84346
Ag	1.28391	0.90748	1.83896
P	2.76724	1.41589	3.76135
C	2.85882	3.19456	4.24914
C	4.00003	3.77990	4.84332
C	4.02577	5.15264	5.13529
C	2.91295	5.95704	4.84096
C	1.77586	5.38289	4.25220
C	1.74950	4.01263	3.95063
Ag	1.36462	-1.94705	0.84513
P	1.18408	-4.46097	0.79860
C	0.84859	-5.22635	2.43645
C	0.03131	-6.35576	2.64807
C	-0.10242	-6.90074	3.93598
C	0.59112	-6.33638	5.01881
C	1.39717	-5.20181	4.81703
C	1.51109	-4.63835	3.53837
Ag	1.36462	1.94692	-0.84505

P	1.18424	4.46089	-0.79873
C	0.84842	5.22622	-2.43656
C	0.03147	6.35591	-2.64795
C	-0.10267	6.90079	-3.93586
C	0.59016	6.33605	-5.01894
C	1.39590	5.20121	-4.81740
C	1.51020	4.63787	-3.53872
P	-1.64639	4.59796	0.67352
C	-2.21366	5.44394	2.21047
C	-1.53562	6.51822	2.82551
C	-2.02419	7.07698	4.01937
C	-3.19716	6.57844	4.60753
C	-3.88752	5.52071	3.99221
C	-3.39782	4.95521	2.80694
C	2.75023	5.28522	-0.25068
C	3.16044	6.54285	-0.73838
C	4.32171	7.14766	-0.23000
C	5.07567	6.50678	0.76819
C	4.66546	5.25647	1.26044
C	3.50978	4.64469	0.75149
Ag	-1.29701	2.09972	0.69515
Ag	-1.10626	-0.64510	1.82305
P	-2.34926	0.01039	3.90666
C	-2.72410	-1.47930	4.92611
C	-3.75801	-1.53008	5.88581
C	-3.93836	-2.67694	6.67296
C	-3.07590	-3.77746	6.52456
C	-2.03840	-3.73261	5.57984
C	-1.86827	-2.59207	4.77791
Ag	-3.25655	0.00005	0.00006
P	-4.75267	-0.61664	-1.89281
C	-5.66242	-2.19869	-1.65308
C	-5.41371	-2.94473	-0.48309
C	-6.03951	-4.18616	-0.28478
C	-6.91560	-4.69100	-1.25655
C	-7.17404	-3.95085	-2.42516
C	-6.55406	-2.70882	-2.62481
Ag	-1.10634	0.64513	-1.82296
P	-2.34946	-0.01040	-3.90655
C	-2.72433	1.47926	-4.92602
C	-1.86879	2.59222	-4.77758
C	-2.03908	3.73280	-5.57942
C	-3.07644	3.77749	-6.52430
C	-3.93859	2.67676	-6.67296
C	-3.75811	1.52987	-5.88589
Ag	-1.29706	-2.09970	-0.69515
P	-1.64667	-4.59794	-0.67343
C	-2.21416	-5.44396	-2.21026
C	-1.53619	-6.51822	-2.82541
C	-2.02498	-7.07702	-4.01917
C	-3.19808	-6.57853	-4.60712
C	-3.88835	-5.52081	-3.99169
C	-3.39845	-4.95527	-2.80651

P	-4.75252	0.61683	1.89307
C	-5.66214	2.19896	1.65340
C	-5.41357	2.94490	0.48331
C	-6.03935	4.18634	0.28501
C	-6.91526	4.69131	1.25688
C	-7.17356	3.95126	2.42558
C	-6.55361	2.70922	2.62522
C	-1.61712	1.16433	5.14991
C	-1.11223	0.70435	6.38397
C	-0.53149	1.60523	7.29035
C	-0.46131	2.97324	6.98637
C	-0.96151	3.43742	5.75937
C	-1.51553	2.53774	4.83794
C	-1.61752	-1.16447	-5.14984
C	-1.11263	-0.70454	-6.38392
C	-0.53202	-1.60547	-7.29033
C	-0.46194	-2.97349	-6.98636
C	-0.96211	-3.43761	-5.75933
C	-1.51601	-2.53788	-4.83787
C	-6.05968	-0.63977	2.19868
C	-7.37430	-0.46704	1.71645
C	-8.32293	-1.49072	1.87003
C	-7.97444	-2.69120	2.50837
C	-6.66675	-2.86830	2.98963
C	-5.71075	-1.85558	2.82777
C	-6.05968	0.64012	-2.19835
C	-7.37414	0.46772	-1.71555
C	-8.32265	1.49154	-1.86897
C	-7.97419	2.69182	-2.50770
C	-6.66667	2.86858	-2.98953
C	-5.71079	1.85572	-2.82785
C	-2.67719	5.37218	-0.64495
C	-2.91554	4.63631	-1.82463
C	-3.69453	5.18772	-2.85368
C	-4.24870	6.47029	-2.71029
C	-4.02116	7.20446	-1.53316
C	-3.23947	6.65922	-0.50293
C	2.48836	0.46704	5.32135
C	2.97649	0.88611	6.57662
C	2.77704	0.08704	7.71342
C	2.08268	-1.13109	7.60999
C	1.57840	-1.54292	6.36627
C	1.77703	-0.74721	5.22742
C	2.48792	-0.46719	-5.32127
C	2.97609	-0.88617	-6.57656
C	2.77652	-0.08709	-7.71334
C	2.08200	1.13095	-7.60986
C	1.57769	1.54266	-6.36611
C	1.77644	0.74694	-5.22728
C	6.71968	0.09551	1.91223
C	7.70998	-0.69707	2.52490
C	9.06645	-0.36232	2.37944
C	9.44288	0.76242	1.62949

C	8.45862	1.55487	1.01490
C	7.10513	1.21913	1.14907
C	-2.67741	-5.37200	0.64518
C	-3.23977	-6.65902	0.50327
C	-4.02137	-7.20420	1.53360
C	-4.24874	-6.46998	2.71072
C	-3.69448	-5.18743	2.85401
C	-2.91558	-4.63608	1.82486
C	2.74995	-5.28536	0.25031
C	3.50958	-4.64472	-0.75174
C	4.66514	-5.25657	-1.26085
C	5.07516	-6.50707	-0.76890
C	4.32113	-7.14805	0.22917
C	3.15999	-6.54315	0.73772
H	-4.71152	2.55747	-0.27058
H	-4.71151	-2.55740	0.27072
H	-0.74932	7.77818	-4.08793
H	-0.51564	6.82070	-1.81505
H	2.57886	7.04753	-1.52546
H	-0.01516	3.67846	7.70360
H	-5.82571	4.75962	-0.62905
H	-7.65981	0.47400	1.22318
H	0.49776	6.77697	-6.02327
H	-4.75108	-2.70755	7.41449
H	3.19508	3.65639	1.12306
H	-4.42612	-0.66770	6.03334
H	-7.65961	-0.47316	-1.22196
H	-0.62480	6.93939	2.37544
H	-6.77052	-2.13172	-3.53760
H	-9.34611	1.34474	-1.49116
H	-3.86259	4.61052	-3.77455
H	-2.49544	3.62303	-1.93193
H	5.24484	4.75306	2.04979
H	-9.34652	-1.34366	1.49266
H	-3.21570	-4.67354	7.14838
H	-1.06023	-2.56470	4.02713
H	-4.68522	-2.02159	3.19181
H	5.98450	6.98530	1.16359
H	-0.01590	-3.67876	-7.70361
H	-5.82574	-4.75952	0.62920
H	-1.48456	7.91408	4.48838
H	-8.72161	3.49008	-2.62948
H	-4.68538	2.02147	-3.19235
H	-7.86591	-4.34468	-3.18539
H	-6.76995	2.13219	3.53809
H	4.64024	8.12750	-0.61753
H	2.13466	3.74150	-3.39061
H	-3.07538	7.23404	0.42175
H	-7.86528	4.34520	3.18590
H	-7.40090	-5.66750	-1.10754
H	-6.38163	-3.80733	3.48753
H	1.94282	4.74846	-5.65835
H	-8.72195	-3.48935	2.63028

H	-1.17378	-0.36095	6.64707
H	-1.06086	2.56497	-4.02668
H	-4.45831	8.20769	-1.41421
H	-3.57529	7.01715	5.54310
H	-1.86729	2.92252	3.86886
H	-3.94619	4.12759	2.33238
H	-3.21636	4.67359	-7.14804
H	-0.91800	4.50734	5.50771
H	-4.75121	2.70725	-7.41462
H	-4.86347	6.89916	-3.51652
H	-6.38160	3.80744	-3.48776
H	-4.42597	0.66733	-6.03360
H	-4.81281	5.12479	4.43728
H	-7.40053	5.66782	1.10787
H	-1.36336	-4.59041	5.44739
H	-1.36426	4.59075	-5.44678
H	-0.13610	1.22855	8.24536
H	-1.17413	0.36076	-6.64705
H	-0.13664	-1.22882	-8.24536
H	-0.91869	-4.50754	-5.50765
H	-1.86772	-2.92265	-3.86878
H	4.89801	-2.91406	1.08569
H	4.89787	2.91447	-1.08663
H	-1.48540	-7.91411	-4.48827
H	-0.62527	-6.93935	-2.37552
H	-3.07580	-7.23387	-0.42141
H	1.92529	-1.75213	8.50518
H	5.08506	-5.16063	2.14640
H	7.42512	-1.57923	3.11780
H	-3.57638	-7.01727	-5.54260
H	4.92184	5.59553	5.59615
H	-2.49544	-3.62281	1.93209
H	4.88649	3.17064	5.07707
H	7.42481	1.57974	-3.11782
H	-0.51634	-6.82022	1.81535
H	4.79240	1.07383	-5.03087
H	9.83445	0.98808	-2.85960
H	5.24458	-4.75308	-2.05010
H	3.19503	-3.65628	-1.12308
H	-3.86240	-4.61021	3.77489
H	9.83476	-0.98732	2.85982
H	2.93569	7.03357	5.06835
H	0.86698	3.56330	3.46882
H	6.33826	1.82789	0.64159
H	-4.86343	-6.89879	3.51704
H	1.92450	1.75200	-8.50501
H	5.08458	5.16084	-2.14792
H	-0.74929	-7.77792	4.08826
H	10.50670	-1.01805	-1.51505
H	6.33802	-1.82778	-0.64214
H	4.88621	3.31532	-6.07672
H	4.79285	-1.07432	5.03036
H	-4.45859	-8.20740	1.41472

H	-3.94676	-4.12766	-2.33188
H	2.57838	-7.04788	1.52475
H	4.88693	-3.31607	6.07566
H	5.06573	5.37684	-4.65108
H	8.74733	2.42703	0.40943
H	-4.81374	-5.12492	-4.43659
H	10.50693	1.01874	1.51514
H	3.50566	1.84611	6.67514
H	0.86673	-3.56351	-3.46911
H	4.63950	-8.12803	0.61647
H	0.49901	-6.77740	6.02312
H	1.37331	-1.06442	4.25303
H	2.13583	-3.74221	3.39008
H	2.93544	-7.03373	-5.06874
H	1.01258	-2.48304	6.27803
H	4.92165	-5.59572	-5.59636
H	5.98390	-6.98566	-1.16445
H	8.74712	-2.42668	-0.40973
H	4.88633	-3.17085	-5.07716
H	1.94462	-4.74934	5.65779
H	5.06649	-5.37722	4.64955
H	0.89775	6.00482	4.02337
H	0.89747	-6.00498	-4.02380
H	3.16184	0.42162	8.68900
H	3.50540	-1.84609	-6.67512
H	3.16136	-0.42158	-8.68893
H	1.01173	2.48271	-6.27784
H	1.37267	1.06408	-4.25289
H	-2.35991	1.57275	-0.71318
H	2.62332	1.61254	0.47761
H	-0.17571	2.00018	2.05116
H	0.64447	-1.02150	2.24683
H	2.62347	-1.61253	-0.47743
H	-0.17571	-2.00036	-2.05114
H	0.64445	1.02121	-2.24671
H	-2.35989	-1.57257	0.71326
C	4.55840	-1.08582	-3.35489
H	4.92457	-2.00900	-2.86060
H	5.18174	-0.92913	-4.25916
C	0.05595	5.30757	0.42838
H	0.04540	6.40192	0.24180
H	0.57949	5.13961	1.39329
C	4.55861	1.08567	3.35475
H	4.92479	2.00896	2.86069
H	5.18195	0.92890	4.25902
C	-3.98378	0.86365	3.58289
H	-4.72232	0.64886	4.38121
H	-3.75634	1.94684	3.63533
C	0.05565	-5.30764	-0.42833
H	0.04500	-6.40200	-0.24176
H	0.57910	-5.13976	-1.39331
C	-3.98395	-0.86366	-3.58259
H	-4.72251	-0.64907	-4.38094

H	-3.75642	-1.94684	-3.63479

Table S19: Cartesian coordinates for $[Ag_{10}H_8(dppm)_6]^{2+}$ via $\mathbf{7b}^{2+}$.

C	-6.25049	-1.97530	-3.67667
C	-5.71741	-1.65649	-2.40515
C	-5.79912	-2.60790	-1.36977
C	-6.42344	-3.84438	-1.59234
C	-6.95411	-4.15243	-2.85305
C	-6.86299	-3.21745	-3.89764
P	-4.89386	-0.04804	-2.04778
P	-2.54967	1.30999	-3.72612
C	-3.06843	3.05536	-3.96602
C	-4.38507	3.47458	-4.24542
C	-4.66813	4.83952	-4.42507
C	-3.64368	5.79503	-4.33267
C	-2.33100	5.38472	-4.04248
C	-2.04662	4.02641	-3.84832
Ag	-3.41669	0.13672	-0.00522
P	-4.99626	0.31505	1.94969
P	-2.72864	-1.05166	3.78617
C	-3.19812	-2.78613	4.19794
C	-2.31481	-3.80165	3.77032
C	-2.57626	-5.14697	4.07015
C	-3.72903	-5.49836	4.79038
C	-4.61555	-4.49674	5.21988
C	-4.34952	-3.14826	4.93163
Ag	-1.36654	-0.96554	1.69297
Ag	1.12349	0.44171	1.97757
P	2.43276	-0.28671	3.99319
C	3.00473	1.09762	5.06606
C	2.30090	2.31690	4.96891
C	2.63876	3.40176	5.79500
C	3.69507	3.28309	6.71223
C	4.40823	2.07497	6.80874
C	4.06045	0.98507	5.99718
Ag	-1.21253	2.03333	1.07363
Ag	-1.22640	1.11562	-1.63253
Ag	1.09391	-0.54423	-1.97815
P	2.49670	0.09464	-3.95993
C	2.95733	-1.33083	-5.03165
C	4.09233	-1.35452	-5.87028
C	4.33868	-2.45991	-6.69827
C	3.44584	-3.54578	-6.71126
C	2.31227	-3.52979	-5.88248
C	2.07499	-2.43281	-5.03816
P	-1.06110	4.60327	1.09607
C	-0.52855	5.27030	2.72175
C	0.38692	6.32751	2.89842
C	0.69985	6.78406	4.18917
C	0.08822	6.20425	5.31233
C	-0.82544	5.14859	5.14474
C	-1.11989	4.67364	3.85875

P	1.70827	4.47497	-0.48235
C	2.29876	5.27823	-2.03450
C	1.57156	6.24763	-2.75766
C	2.09960	6.79413	-3.94077
C	3.35302	6.38044	-4.41636
C	4.08373	5.41741	-3.70008
C	3.56155	4.86911	-2.52125
C	2.83776	5.18447	0.79296
C	3.40333	6.47035	0.65209
C	4.24781	6.98142	1.64919
C	4.53809	6.21157	2.78958
C	3.98327	4.92912	2.92885
C	3.13646	4.41350	1.93478
Ag	1.44148	2.00467	-0.48272
Ag	3.27091	-0.16323	0.01785
P	4.83525	0.52107	-1.79943
C	-2.54862	5.61753	0.67338
C	-2.88781	6.80961	1.34779
C	-4.00194	7.55873	0.93391
C	-4.77916	7.12874	-0.15461
C	-4.44459	5.94190	-0.82791
C	-3.33992	5.18306	-0.41256
Ag	1.20002	-2.12360	0.49042
P	1.18713	-4.60536	0.41454
P	-1.60891	-4.41704	-1.12798
C	-1.18309	-5.06993	-2.78999
C	-0.39201	-6.21194	-3.02938
C	-0.11932	-6.61931	-4.34541
C	-0.64385	-5.90068	-5.43205
C	-1.43161	-4.75873	-5.20225
C	-1.68896	-4.33914	-3.88955
Ag	-1.42217	-1.86796	-1.04912
C	-2.09737	-0.35287	5.37932
C	-2.40092	-0.89443	6.64445
C	-1.98241	-0.23539	7.81153
C	-1.24765	0.95757	7.72779
C	-0.91543	1.48360	6.46877
C	-1.33486	0.83329	5.29836
P	4.72621	-0.98691	1.86430
C	6.11118	0.17357	2.20914
C	7.39703	-0.04275	1.66925
C	8.40841	0.91457	1.84790
C	8.15343	2.09120	2.56959
C	6.87465	2.31257	3.10672
C	5.85552	1.36826	2.91811
C	-6.26545	1.18737	-1.94333
C	-7.55991	0.95247	-2.45356
C	-8.57812	1.89930	-2.25740
C	-8.31941	3.08194	-1.54368
C	-7.03259	3.32354	-1.03596
C	-6.01078	2.38362	-1.23804
C	5.54532	-2.60733	1.55284
C	5.23996	-3.29226	0.35970

C	5.78761	-4.56066	0.10723
C	6.64265	-5.15320	1.04765
C	6.95964	-4.47323	2.23833
C	6.41749	-3.20487	2.49158
C	1.64792	-1.45859	5.18733
C	1.43843	-1.14464	6.54550
C	0.83151	-2.07847	7.40015
C	0.42761	-3.33102	6.91416
C	0.62111	-3.64433	5.55939
C	1.21528	-2.71161	4.69781
C	6.07281	-0.78336	-2.19142
C	7.42702	-0.67076	-1.81142
C	8.31674	-1.73258	-2.04307
C	7.87061	-2.91086	-2.66139
C	6.52256	-3.03008	-3.03763
C	5.62561	-1.98151	-2.79182
C	5.82361	2.04228	-1.47986
C	5.60579	2.74020	-0.27512
C	6.27679	3.94773	-0.02185
C	7.16887	4.46644	-0.97148
C	7.39809	3.77300	-2.17420
C	6.73091	2.56616	-2.42969
C	-1.94171	0.76258	-5.38337
C	-2.24775	1.44451	-6.57740
C	-1.90788	0.87556	-7.81567
C	-1.26347	-0.37049	-7.87085
C	-0.93165	-1.03919	-6.68081
C	-1.26139	-0.47406	-5.43998
C	1.87951	1.34933	-5.17096
C	1.74325	1.08179	-6.54794
C	1.28085	2.08008	-7.41979
C	0.95195	3.35319	-6.93172
C	1.07518	3.62244	-5.55954
C	1.52431	2.62617	-4.68124
C	2.24731	-5.40486	-0.86647
C	2.69927	-6.73528	-0.72994
C	3.49337	-7.31578	-1.73053
C	3.84461	-6.57220	-2.87095
C	3.40043	-5.24697	-3.00737
C	2.60583	-4.66101	-2.00912
C	1.68459	-5.47467	1.96458
C	0.89302	-6.43158	2.63486
C	1.34741	-7.01875	3.82895
C	2.59528	-6.66463	4.36406
C	3.39402	-5.72085	3.69658
C	2.94112	-5.12763	2.51077
C	-3.16540	-5.29532	-0.65409
C	-3.75440	-4.91899	0.57375
C	-4.83090	-5.65170	1.09391
C	-5.35896	-6.73649	0.37189
C	-4.81072	-7.07789	-0.87573
C	-3.71135	-6.36756	-1.38670
C	-6.42189	-0.81966	1.71102

C	-7.50262	-0.41209	0.89512
C	-8.54439	-1.30315	0.60250
C	-8.52553	-2.61090	1.11400
C	-7.45039	-3.02514	1.91514
C	-6.39948	-2.14062	2.20601
C	-5.76409	1.95096	2.31925
C	-4.99702	3.10604	2.06290
C	-5.49241	4.37517	2.39906
C	-6.76479	4.50085	2.97916
C	-7.53479	3.35434	3.23611
C	-7.03566	2.08246	2.91708
H	-5.36571	-2.38312	-0.38343
H	-4.00847	3.01042	1.58218
H	0.71981	-7.76540	4.33942
H	-0.07951	-6.74487	2.22784
H	2.44015	-7.31719	0.16844
H	-1.00564	-0.81454	-8.84441
H	-6.47961	-4.57393	-0.77345
H	-7.78678	0.01350	-2.97994
H	2.94608	-7.12523	5.29963
H	-5.70042	5.15460	-4.64115
H	2.26814	-3.61665	-2.11044
H	-5.20504	2.74526	-4.32031
H	-7.53568	0.60886	0.48756
H	0.03037	-6.79041	-2.19496
H	-7.64329	1.18992	3.12991
H	-9.37670	-0.96803	-0.03471
H	-5.25482	-5.36987	2.06939
H	-3.36062	-4.05532	1.13445
H	3.66683	-4.66164	-3.89940
H	-9.58652	1.70288	-2.65276
H	-3.87006	6.86214	-4.47708
H	-1.02086	3.70325	-3.60948
H	-5.01023	2.56590	-0.81566
H	4.47085	-7.02752	-3.65355
H	-0.91990	1.46952	8.64539
H	-4.88635	5.26802	2.19211
H	0.50734	-7.50719	-4.51862
H	-9.34575	-3.30718	0.88389
H	-5.55769	-2.49424	2.81814
H	-8.53071	3.44853	3.69529
H	-6.19279	-1.25615	-4.50765
H	3.84460	-8.35271	-1.61630
H	3.57778	-4.39394	1.99394
H	-3.26745	-6.66032	-2.35055
H	-7.27280	-3.45432	-4.89137
H	-7.15786	5.49733	3.23207
H	-6.82268	4.23260	-0.45264
H	4.37799	-5.43693	4.09937
H	-9.12648	3.81060	-1.37339
H	-2.76290	2.41679	-6.54219
H	-1.41215	-3.52380	3.20115
H	-5.22978	-7.91773	-1.45078

H	-0.43822	-6.23060	-6.46198
H	-0.98798	-0.98964	-4.50424
H	-2.28923	-3.43163	-3.71057
H	-3.93838	-6.55443	5.01834
H	-0.39559	-2.00006	-6.71440
H	-5.51822	-4.76446	5.78992
H	-6.20472	-7.31194	0.77807
H	-7.42482	-4.04855	2.31945
H	-5.05137	-2.37859	5.28810
H	-1.84218	-4.18627	-6.04798
H	-7.43385	-5.12786	-3.02573
H	-1.52299	6.12846	-3.96275
H	-1.87464	-5.92568	3.73547
H	-2.15441	1.41087	-8.74537
H	-2.96331	-1.83606	6.72694
H	-2.23099	-0.66331	8.79477
H	-0.30861	2.39817	6.39242
H	-1.05374	1.23642	4.31159
H	4.89083	2.34208	0.46104
H	4.55222	-2.83361	-0.36719
H	1.42429	7.60319	4.31252
H	0.87318	6.80225	2.03446
H	-2.28120	7.15408	2.19920
H	0.59621	4.13518	-7.61946
H	6.08503	4.48570	0.91807
H	7.78960	0.25019	-1.33148
H	0.32334	6.57507	6.32175
H	5.23047	-2.47038	-7.34313
H	-3.08929	4.24690	-0.93877
H	4.79355	-0.50635	-5.88550
H	7.61055	-0.96467	1.10790
H	0.59211	6.60072	-2.40342
H	6.68055	-2.67500	3.42066
H	9.40796	0.73347	1.42365
H	4.20491	4.32212	3.81867
H	2.71125	3.40186	2.03765
H	-5.04346	5.59626	-1.68263
H	9.37096	-1.63254	-1.74233
H	3.63867	-4.40810	-7.36765
H	1.19868	-2.43194	-4.36847
H	4.56582	-2.10601	-3.06098
H	-5.64961	7.71986	-0.47740
H	-0.04131	-4.06253	7.58955
H	5.52916	-5.08604	-0.82406
H	1.52407	7.55448	-4.49092
H	8.95059	2.83623	2.71158
H	4.85353	1.57192	3.32400
H	7.63671	-4.93496	2.97330
H	6.92256	2.02781	-3.37120
H	-4.26124	8.48700	1.46557
H	-1.82150	3.83236	3.73265
H	3.19178	7.07131	-0.24624
H	8.10248	4.17627	-2.91790

H	7.06701	-6.15051	0.85619
H	6.15894	-3.95259	-3.51493
H	-1.30966	4.68872	6.01948
H	8.57240	-3.73802	-2.84594
H	1.99871	0.09033	-6.94784
H	1.48318	2.41432	4.23540
H	4.68678	7.98407	1.53234
H	3.76088	6.80883	-5.34405
H	1.59841	2.84976	-3.60575
H	4.14951	4.12542	-1.96228
H	3.96698	4.13415	7.35526
H	0.82701	4.61795	-5.16440
H	5.23659	1.97853	7.52696
H	5.20467	6.61219	3.56874
H	6.66195	3.23303	3.67159
H	4.61671	0.04042	6.09879
H	5.07038	5.08557	-4.05706
H	7.68926	5.41681	-0.77824
H	1.61229	-4.37866	-5.87178
H	2.07689	4.34351	5.70446
H	1.17820	1.85544	-8.49202
H	1.74903	-0.16838	6.94383
H	0.67615	-1.81969	8.45815
H	0.31242	-4.62293	5.16460
H	1.34234	-2.96844	3.63494
H	-0.35298	-1.56450	-2.42832
H	-2.44199	1.78399	-0.27994
H	-0.15094	1.66236	2.43816
H	-2.59890	-1.57137	0.34285
H	0.50768	1.52076	-1.96004
H	2.35096	-1.59339	-0.87957
H	2.50336	1.36781	0.89852
H	0.34596	-1.50924	1.97624
C	0.07873	5.32427	-0.19348
H	-0.49814	5.17537	-1.13086
H	0.19885	6.41820	-0.04558
C	3.95492	-1.28408	3.54506
H	4.72325	-1.24273	4.34368
H	3.58989	-2.33025	3.49826
C	4.08585	0.94613	-3.46206
H	4.84776	0.89653	-4.26638
H	3.79275	2.01148	-3.36070
C	-0.50988	-5.29620	0.10134
H	-1.05937	-5.15356	1.05469
H	-0.48294	-6.38719	-0.10307
C	-4.09765	0.28221	-3.70475
H	-4.83173	0.63923	-4.45587
H	-3.74229	-0.71101	-4.04797
C	-4.32278	-0.07844	3.65678
H	-5.12857	-0.47447	4.30903
H	-4.05288	0.91668	4.06456

Table S20: Cartesian coordinates for $[Ag_{10}H_8(dppa)_6]^{2+}$ via $\mathbf{4a}^{2+}$.

Ag	0.83003300000000	-2.30608500000000	0.40245200000000
Ag	-0.41094900000000	0.56463400000000	1.87997800000000
Ag	1.91357000000000	1.68003400000000	-0.61754800000000
Ag	3.14394400000000	-0.88310900000000	-0.99514600000000
Ag	-3.12646000000000	0.87474100000000	0.98055800000000
Ag	-1.97108600000000	-1.72621400000000	0.60895000000000
Ag	0.44449400000000	-0.63218400000000	-1.94364300000000
Ag	-0.88230000000000	2.25993500000000	-0.49592500000000
Ag	-2.20837200000000	-0.02490500000000	-1.59058300000000
Ag	2.21801600000000	-0.08448500000000	1.53526100000000
P	2.29077500000000	4.07783000000000	-0.92514200000000
P	-0.60191400000000	4.42823000000000	-1.73275500000000
P	1.36235700000000	-1.44915100000000	-4.08003200000000
P	4.17776900000000	-1.83596200000000	-3.02702300000000
P	-2.44446700000000	-4.10761600000000	0.94635300000000
P	0.50352600000000	-4.54054700000000	1.46029800000000
P	-4.00537900000000	1.75366900000000	3.14876500000000
P	-1.16881700000000	1.37453000000000	4.06997500000000
P	-4.09370900000000	0.56047100000000	-2.95681900000000
P	4.10634900000000	-0.60643500000000	2.91033800000000
P	-6.91797800000000	-0.72853800000000	-2.63319500000000
P	6.78009700000000	1.01198000000000	2.80976300000000
C	-4.86917300000000	0.61884400000000	4.29720600000000
C	-1.51611400000000	0.01425500000000	5.26896500000000
C	-1.30246500000000	5.91680600000000	-0.90840000000000
C	2.35893300000000	5.14169100000000	0.57941000000000
C	5.25300100000000	-0.77098700000000	-4.06687800000000
C	1.09789300000000	-5.96846400000000	0.46743700000000
C	-2.74184700000000	-5.13280400000000	-0.55655300000000
C	-3.89945200000000	-4.49259400000000	1.99641200000000
C	1.28153700000000	-4.68348800000000	3.11014600000000
C	-0.01074600000000	2.48208100000000	4.96516600000000
C	-4.98706400000000	3.30256500000000	3.06773700000000
C	-1.21765600000000	4.46784200000000	-3.45769500000000
C	3.83800800000000	4.48349200000000	-1.82147800000000
C	0.23975200000000	-2.59976700000000	-4.96509100000000
C	5.07199000000000	-3.41840600000000	-2.80757000000000
C	-4.97280100000000	0.89393200000000	5.67751400000000
C	-5.58542300000000	-0.03490600000000	6.52938800000000
C	-6.09247800000000	-1.24006300000000	6.01084500000000
C	-5.97913500000000	-1.52254700000000	4.64080600000000
C	-5.36007200000000	-0.59925400000000	3.78447600000000
H	-4.54743200000000	1.82576900000000	6.08013000000000
H	-5.66119900000000	0.17737300000000	7.60663400000000
H	-6.56751800000000	-1.96949900000000	6.68460300000000
H	-6.34797100000000	-2.47560500000000	4.23554400000000
H	-5.22301500000000	-0.83836800000000	2.71704800000000
C	-1.35980100000000	0.16253900000000	6.66286000000000
C	-1.68795400000000	-0.89646900000000	7.52246600000000
C	-2.18861700000000	-2.10217600000000	7.00048000000000
C	-2.34544500000000	-2.25377600000000	5.61368200000000

C	-1.99301500000000	-1.20673100000000	4.74865700000000
H	-0.97323500000000	1.10466700000000	7.07957200000000
H	-1.55882000000000	-0.77745800000000	8.60910700000000
H	-2.46041800000000	-2.92454700000000	7.68006300000000
H	-2.75529700000000	-3.18561800000000	5.19667400000000
H	-2.09493800000000	-1.33656000000000	3.65841200000000
C	-1.64554600000000	7.10227900000000	-1.59319800000000
C	-2.09385500000000	8.22264700000000	-0.87630200000000
C	-2.19050300000000	8.17439200000000	0.52484700000000
C	-1.84322700000000	6.99946400000000	1.21259400000000
C	-1.41117800000000	5.87209800000000	0.49853400000000
H	-1.56864300000000	7.14975500000000	-2.69061400000000
H	-2.36460700000000	9.14302000000000	-1.41568300000000
H	-2.53582300000000	9.05833200000000	1.08254200000000
H	-1.91284800000000	6.95837600000000	2.31027400000000
H	-1.14252600000000	4.94627300000000	1.03299000000000
C	2.83224700000000	6.47050100000000	0.51890300000000
C	2.72231200000000	7.30657600000000	1.63917800000000
C	2.14596900000000	6.82104800000000	2.82723600000000
C	1.68831700000000	5.49558800000000	2.89705100000000
C	1.79642100000000	4.65454700000000	1.77705500000000
H	3.29395300000000	6.85240000000000	-0.40598700000000
H	3.09061200000000	8.34251700000000	1.58744800000000
H	2.06087000000000	7.47961200000000	3.70519700000000
H	1.24923200000000	5.10828200000000	3.82808300000000
H	1.43815400000000	3.61332700000000	1.83278400000000
C	1.61389500000000	-0.07897100000000	-5.29370200000000
C	1.26961500000000	-0.16972000000000	-6.65938400000000
C	1.57495000000000	0.88706100000000	-7.53183700000000
C	2.23678100000000	2.03090100000000	-7.05293400000000
C	2.57557800000000	2.12812300000000	-5.69182600000000
C	2.24803000000000	1.08754900000000	-4.81162100000000
H	0.75996900000000	-1.06717600000000	-7.04303700000000
H	1.30448900000000	0.81099800000000	-8.59680200000000
H	2.49033500000000	2.84862000000000	-7.74479300000000
H	3.10080600000000	3.01611200000000	-5.30809300000000
H	2.48914500000000	1.17956800000000	-3.73851200000000
C	5.80547000000000	-1.21739100000000	-5.28690000000000
C	6.53167500000000	-0.33109900000000	-6.09449600000000
C	6.71307400000000	1.00423900000000	-5.69016400000000
C	6.16910400000000	1.45344400000000	-4.47726800000000
C	5.43668400000000	0.56995500000000	-3.66875900000000
H	5.67698000000000	-2.26480300000000	-5.60664000000000
H	6.96028900000000	-0.68268800000000	-7.04481700000000
H	7.28363800000000	1.69680500000000	-6.32741700000000
H	6.30338500000000	2.49716200000000	-4.15569600000000
H	4.99503600000000	0.92193100000000	-2.72166400000000
C	-3.25642700000000	-6.44385200000000	-0.45445100000000
C	-3.34658000000000	-7.25456700000000	-1.59467600000000
C	-2.93047200000000	-6.75978100000000	-2.84388300000000
C	-2.43123300000000	-5.45222100000000	-2.95236000000000
C	-2.33828500000000	-4.63657700000000	-1.81261700000000
H	-3.59637900000000	-6.83123500000000	0.51963700000000

H	-3.74619100000000	-8.27665200000000	-1.51000600000000
H	-3.00095300000000	-7.39768100000000	-3.73823500000000
H	-2.11023800000000	-5.05898500000000	-3.92738600000000
H	-1.94316300000000	-3.61072100000000	-1.89933600000000
C	1.53792800000000	-7.18629500000000	1.02747600000000
C	1.89367300000000	-8.25473600000000	0.18912000000000
C	1.79979000000000	-8.12053900000000	-1.20686900000000
C	1.35919300000000	-6.91012300000000	-1.76940700000000
C	1.02212800000000	-5.83350300000000	-0.93663600000000
H	1.60820700000000	-7.29910100000000	2.12078000000000
H	2.24012900000000	-9.20204800000000	0.62961200000000
H	2.07091100000000	-8.96503200000000	-1.85880600000000
H	1.28199100000000	-6.79938900000000	-2.86194300000000
H	0.69108200000000	-4.87842200000000	-1.37671300000000
C	-5.17704600000000	-4.18541400000000	1.47710200000000
C	-6.32720000000000	-4.45859200000000	2.23045700000000
C	-6.21630900000000	-5.03069500000000	3.51040700000000
C	-4.94823900000000	-5.31693100000000	4.03900600000000
C	-3.79136800000000	-5.04788000000000	3.28764100000000
H	-5.28144200000000	-3.75667200000000	0.46741500000000
H	-7.31436200000000	-4.23051000000000	1.80239400000000
H	-7.12134100000000	-5.25501300000000	4.09527300000000
H	-4.85538800000000	-5.76278000000000	5.04094900000000
H	-2.80074800000000	-5.28123700000000	3.70577800000000
C	2.67712600000000	-4.87407500000000	3.22172300000000
C	3.28777100000000	-4.85489500000000	4.48471000000000
C	2.52257800000000	-4.62766700000000	5.64056500000000
C	1.13873300000000	-4.41616300000000	5.53090100000000
C	0.51905500000000	-4.43942800000000	4.27289200000000
H	3.29432700000000	-5.03462200000000	2.32373400000000
H	4.37385100000000	-5.00883200000000	4.55910700000000
H	3.00854400000000	-4.60378600000000	6.62739200000000
H	0.53261600000000	-4.22288600000000	6.42938200000000
H	-0.56154200000000	-4.25612800000000	4.18514500000000
C	-6.23850100000000	3.45570500000000	3.69796500000000
C	-6.95790900000000	4.65255900000000	3.54596900000000
C	-6.43317600000000	5.70370800000000	2.77656500000000
C	-5.18509700000000	5.55562600000000	2.14652300000000
C	-4.47059900000000	4.35595900000000	2.27775200000000
H	-6.65160100000000	2.63985000000000	4.31046500000000
H	-7.93437600000000	4.76614400000000	4.04126600000000
H	-6.99910800000000	6.64115900000000	2.66673700000000
H	-4.76453700000000	6.37158600000000	1.53830200000000
H	-3.51246400000000	4.23272700000000	1.74607100000000
C	1.37033400000000	2.27763000000000	4.75924700000000
C	2.31111400000000	3.03733500000000	5.46930600000000
C	1.88258200000000	4.02162700000000	6.37513300000000
C	0.50888900000000	4.24312000000000	6.57114700000000
C	-0.43864000000000	3.47212400000000	5.87728500000000
H	1.71080000000000	1.52174500000000	4.03455600000000
H	3.38383500000000	2.85757900000000	5.30648300000000
H	2.62114000000000	4.62206700000000	6.92757200000000
H	0.16967200000000	5.01372600000000	7.28000000000000

H	-1.51251300000000	3.62958100000000	6.06266000000000
C	-2.57802100000000	4.72923300000000	-3.73547400000000
C	-3.04595300000000	4.67116400000000	-5.05628500000000
C	-2.17532800000000	4.33394900000000	-6.10510000000000
C	-0.83005900000000	4.04201800000000	-5.82828200000000
C	-0.35188000000000	4.10471400000000	-4.51213700000000
H	-3.27891100000000	4.98081100000000	-2.92424700000000
H	-4.10448500000000	4.88718900000000	-5.26096100000000
H	-2.55004100000000	4.28727200000000	-7.13793600000000
H	-0.14180100000000	3.75612200000000	-6.63820900000000
H	0.69955100000000	3.86638200000000	-4.29627100000000
C	5.06088600000000	4.26461400000000	-1.14748800000000
C	6.27775600000000	4.50531400000000	-1.80031500000000
C	6.28882900000000	4.96391100000000	-3.12981700000000
C	5.07660600000000	5.16988400000000	-3.80735900000000
C	3.85323200000000	4.92633200000000	-3.15999200000000
H	5.06758700000000	3.92457200000000	-0.09939700000000
H	7.21975800000000	4.34192100000000	-1.25602400000000
H	7.24516700000000	5.16438000000000	-3.63639200000000
H	5.07963700000000	5.52905000000000	-4.84777200000000
H	2.90710700000000	5.08581000000000	-3.69858500000000
C	-1.13329400000000	-2.28712400000000	-4.93586900000000
C	-2.05474800000000	-3.04742500000000	-5.66915100000000
C	-1.61698000000000	-4.14072700000000	-6.42706400000000
C	-0.25733200000000	-4.48041000000000	-6.43112300000000
C	0.66928100000000	-3.71593200000000	-5.70256000000000
H	-1.48701300000000	-1.43965700000000	-4.33464500000000
H	-3.11878400000000	-2.77840800000000	-5.64217400000000
H	-2.33807200000000	-4.73609700000000	-7.00723200000000
H	0.08914500000000	-5.34238100000000	-7.01393700000000
H	1.72854600000000	-4.00196500000000	-5.72015000000000
C	6.48221400000000	-3.49043500000000	-2.82938600000000
C	7.12827800000000	-4.69682800000000	-2.51408300000000
C	6.37728500000000	-5.83346600000000	-2.16931200000000
C	4.97199300000000	-5.76219300000000	-2.13459300000000
C	4.32025900000000	-4.56134600000000	-2.44813100000000
H	7.07731600000000	-2.60259600000000	-3.09188700000000
H	8.22829800000000	-4.74746400000000	-2.53999200000000
H	6.88830200000000	-6.77708200000000	-1.92475600000000
H	4.37322900000000	-6.64330400000000	-1.85482800000000
H	3.22091800000000	-4.50497900000000	-2.40930200000000
C	-3.85789100000000	0.36132900000000	-4.76232800000000
C	-4.98845500000000	2.15863800000000	-2.78300600000000
C	-7.13062700000000	-2.46190800000000	-2.02311700000000
C	-7.50709600000000	0.27708400000000	-1.18895800000000
C	3.76489300000000	-0.51434300000000	4.70663500000000
C	5.16016300000000	-2.09302200000000	2.67382600000000
C	7.58287800000000	0.25317300000000	1.31847200000000
C	6.79387600000000	2.81366900000000	2.38773900000000
C	2.56105400000000	-1.10172200000000	5.15375000000000
C	2.19290900000000	-1.01450100000000	6.50420600000000
C	3.02021800000000	-0.33738200000000	7.41501000000000
C	4.22105200000000	0.24504700000000	6.97542100000000

C	4.59686700000000	0.16072500000000	5.62506500000000
H	1.89867000000000	-1.61801000000000	4.43902300000000
H	1.24446400000000	-1.46182100000000	6.83731700000000
H	2.72609900000000	-0.25728700000000	8.47265700000000
H	4.87122600000000	0.77404800000000	7.68879800000000
H	5.53768800000000	0.62186600000000	5.28362800000000
C	5.96444000000000	-2.62276700000000	3.70411100000000
C	6.80686600000000	-3.71573700000000	3.44279600000000
C	6.84776700000000	-4.28767700000000	2.15966300000000
C	6.04359700000000	-3.76761300000000	1.13066100000000
C	5.20139100000000	-2.67842400000000	1.39122600000000
H	5.93099700000000	-2.18284400000000	4.71254900000000
H	7.43580900000000	-4.12352700000000	4.24905800000000
H	7.50899700000000	-5.14477800000000	1.95988100000000
H	6.06861200000000	-4.21018200000000	0.12400300000000
H	4.56010500000000	-2.28049500000000	0.58467100000000
C	5.68944600000000	3.63448800000000	2.71294400000000
C	5.73197300000000	5.01731600000000	2.47462300000000
C	6.87905800000000	5.60246700000000	1.91584700000000
C	7.98698000000000	4.79691800000000	1.60147200000000
C	7.94775300000000	3.41345700000000	1.83499700000000
H	4.78157500000000	3.18714100000000	3.14561000000000
H	4.85506400000000	5.63564600000000	2.71852700000000
H	6.91051700000000	6.68557500000000	1.72417100000000
H	8.89223800000000	5.24919900000000	1.16785100000000
H	8.81984200000000	2.79310700000000	1.57491500000000
C	8.46404100000000	-0.82274900000000	1.54941400000000
C	9.04385900000000	-1.51447200000000	0.47327300000000
C	8.74985600000000	-1.12965600000000	-0.84301800000000
C	7.87318600000000	-0.05611600000000	-1.08468400000000
C	7.28815300000000	0.63020100000000	-0.01098000000000
H	8.68658000000000	-1.12878000000000	2.58411900000000
H	9.72759600000000	-2.35487600000000	0.66675700000000
H	9.21140200000000	-1.66264500000000	-1.68860300000000
H	7.64803400000000	0.24959500000000	-2.11739800000000
H	6.60256900000000	1.47009300000000	-0.21194000000000
C	-5.71815900000000	2.73132000000000	-3.84518200000000
C	-6.42902400000000	3.92564900000000	-3.64527200000000
C	-6.41553800000000	4.55517600000000	-2.38964400000000
C	-5.69125100000000	3.98749900000000	-1.32716200000000
C	-4.97584000000000	2.79955400000000	-1.52653600000000
H	-5.72984800000000	2.24451700000000	-4.83207100000000
H	-6.99998100000000	4.36560200000000	-4.47738400000000
H	-6.97619500000000	5.48987600000000	-2.23639200000000
H	-5.68453600000000	4.46497000000000	-0.33667200000000
H	-4.39988600000000	2.36371300000000	-0.69151900000000
C	-2.70225400000000	0.94453600000000	-5.32789900000000
C	-2.44323800000000	0.80631500000000	-6.69949800000000
C	-3.33339500000000	0.08660900000000	-7.51396300000000
C	-4.48649900000000	-0.49226200000000	-6.95520300000000
C	-4.75081400000000	-0.36153500000000	-5.58208000000000
H	-1.99295000000000	1.50035400000000	-4.69156800000000
H	-1.53099400000000	1.25240000000000	-7.12460100000000

H	-3.12703400000000	-0.02848600000000	-8.58888100000000
H	-5.18746800000000	-1.05305800000000	-7.59245800000000
H	-5.65642900000000	-0.81463000000000	-5.14756600000000
C	-8.33133000000000	1.38373200000000	-1.47500900000000
C	-8.71205800000000	2.27266000000000	-0.45588400000000
C	-8.26846300000000	2.06095600000000	0.85725200000000
C	-7.45606500000000	0.95154700000000	1.15463300000000
C	-7.07648600000000	0.06273700000000	0.13935600000000
H	-8.65823100000000	1.56223700000000	-2.51181000000000
H	-9.34833900000000	3.13862900000000	-0.69361600000000
H	-8.54985100000000	2.76288100000000	1.65672400000000
H	-7.12123100000000	0.77807400000000	2.18832800000000
H	-6.43785400000000	-0.80277700000000	0.38253700000000
C	-6.19234500000000	-3.46122400000000	-2.37279900000000
C	-6.39780500000000	-4.79700700000000	-1.99305400000000
C	-7.54755900000000	-5.15707800000000	-1.27171500000000
C	-8.49093400000000	-4.17259700000000	-0.93005500000000
C	-8.28561700000000	-2.83408000000000	-1.29945900000000
H	-5.28784800000000	-3.19300900000000	-2.94037200000000
H	-5.64611900000000	-5.55641000000000	-2.25774100000000
H	-7.70761100000000	-6.20390700000000	-0.97263200000000
H	-9.39703600000000	-4.44773400000000	-0.36798500000000
H	-9.02726900000000	-2.07084100000000	-1.01527700000000
H	-2.17364300000000	2.39679800000000	0.70703600000000
H	1.15796800000000	1.43202800000000	1.31967400000000
H	0.30964600000000	1.23446100000000	-1.60092400000000
H	3.54982300000000	0.83294800000000	-0.63524600000000
H	-1.11598400000000	-1.51136400000000	-1.36652200000000
H	2.18698800000000	-2.40849800000000	-0.72238400000000
H	-3.57270500000000	-0.82290000000000	0.58311000000000
H	-0.34162300000000	-1.30064900000000	1.53655700000000
N	-1.16070900000000	-4.92243800000000	1.78445200000000
H	-1.33408400000000	-5.91673800000000	1.99554800000000
N	5.06767800000000	0.75428900000000	2.49300100000000
H	4.71449200000000	1.19038100000000	1.62776600000000
N	-2.65738000000000	2.31387700000000	4.12947600000000
H	-2.49869400000000	3.32516400000000	4.02876300000000
N	-5.16541000000000	-0.67584800000000	-2.43757800000000
H	-4.81029500000000	-1.12202000000000	-1.57820700000000
N	1.08134600000000	4.82040300000000	-1.92650600000000
H	1.26181900000000	5.80326000000000	-2.18051500000000
N	2.86799000000000	-2.31440300000000	-4.06312600000000
H	3.16231600000000	-2.71083000000000	-4.96485600000000

Table S21: Cartesian coordinates for $[Ag_{10}H_8(dppa)_6]^{2+}$ via $\mathbf{4b}^{2+}$.

P	3.24029400000000	1.85698500000000	3.30809700000000
C	3.98651900000000	3.38755400000000	3.98210500000000
P	1.29161500000000	-0.14277500000000	4.30435800000000
C	-0.08975000000000	0.04189100000000	5.50847300000000
C	2.32998700000000	-1.43273100000000	5.10314400000000
Ag	0.42038300000000	-0.37634400000000	1.94607000000000
Ag	-1.14012800000000	1.88817900000000	0.46343800000000
P	-1.01176200000000	4.44471000000000	0.17376000000000
C	-2.64516800000000	5.28292000000000	0.31522700000000
C	4.54383600000000	0.56386600000000	3.45030300000000
Ag	2.00436500000000	1.91878500000000	1.19359900000000
Ag	2.37933600000000	-0.18256700000000	-0.64716000000000
P	3.99370700000000	-0.54717000000000	-2.49846200000000
C	3.92299600000000	-1.95891700000000	-3.67422400000000
Ag	1.09787500000000	2.05702300000000	-1.62911900000000
Ag	-0.16426200000000	-0.56718100000000	-2.09582300000000
Ag	-2.89830000000000	-0.07519400000000	-0.94034200000000
P	-3.69508400000000	0.41318800000000	-3.27491900000000
C	-5.44195300000000	-0.02652600000000	-3.63678300000000
Ag	-2.35689400000000	-0.55869900000000	1.85628900000000
Ag	-1.40627100000000	-2.44442100000000	-0.03680200000000
P	-1.30117100000000	-4.64797300000000	1.14791300000000
C	-1.50075300000000	-4.53089400000000	2.97110000000000
P	-4.15050600000000	0.72276900000000	2.81539100000000
C	-3.74561200000000	2.38283900000000	3.48763200000000
P	-7.02305600000000	0.71106200000000	1.59494700000000
C	-7.16036400000000	-0.91912500000000	0.71764600000000
C	-5.10437700000000	-0.08204400000000	4.16271600000000
P	0.95942400000000	4.45939100000000	-2.10387300000000
C	2.37961400000000	5.51911200000000	-1.56869000000000
C	0.73839100000000	4.93386300000000	-3.86190200000000
P	-1.44265100000000	-1.41158000000000	-4.14595800000000
C	-2.03711600000000	-3.14569100000000	-4.16532000000000
Ag	1.40133200000000	-2.65689500000000	-0.25239200000000
P	1.52429600000000	-5.06657100000000	0.03937300000000
C	2.99246000000000	-5.66991800000000	0.97523600000000
C	-0.46530300000000	-1.24366400000000	-5.69430300000000
C	1.47251800000000	-6.23277000000000	-1.38275900000000
C	4.28960100000000	0.90278500000000	-3.59266800000000
P	7.10481700000000	-0.38531300000000	-2.01428400000000
C	7.84302800000000	-1.56428600000000	-0.78885300000000
C	-2.59638300000000	-5.85075500000000	0.63896000000000
C	-3.55365400000000	2.17586100000000	-3.76133900000000
C	0.05208500000000	5.26205500000000	1.43114200000000
C	-7.50237600000000	1.90249200000000	0.26016100000000
C	7.44074900000000	1.25542800000000	-1.20716500000000
H	-3.04681500000000	-1.82288400000000	-0.47970800000000
H	-0.87283800000000	-1.66451800000000	1.84902000000000
H	0.19246200000000	1.53806200000000	1.67261100000000
H	-2.74188200000000	1.58093400000000	-0.28819500000000
H	-0.06397800000000	-2.26630600000000	-1.39507400000000

H	-0.03996600000000	1.12416100000000	-2.62472900000000
H	2.40659600000000	-1.45295400000000	0.67474000000000
H	2.63706500000000	1.73524500000000	-0.51757400000000
C	-2.78412500000000	-4.43864300000000	3.55205500000000
C	-2.91613400000000	-4.28956500000000	4.94150100000000
C	-1.77652600000000	-4.21543300000000	5.76005600000000
C	-0.49792300000000	-4.27528700000000	5.18334200000000
C	-0.35981200000000	-4.42946500000000	3.79567100000000
H	-3.68410300000000	-4.50560200000000	2.91984200000000
H	-3.91903900000000	-4.23241300000000	5.38970200000000
H	-1.88614700000000	-4.09789700000000	6.84845700000000
H	0.40289100000000	-4.19393900000000	5.81091200000000
H	0.64493100000000	-4.47564800000000	3.35042500000000
C	-2.86927700000000	-7.02507800000000	1.37598700000000
C	-3.85487000000000	-7.91899000000000	0.93402000000000
C	-4.58127000000000	-7.64353400000000	-0.23873000000000
C	-4.31433900000000	-6.47834400000000	-0.97428200000000
C	-3.32107000000000	-5.58463800000000	-0.54128700000000
H	-2.32320800000000	-7.23260500000000	2.31042400000000
H	-4.06631200000000	-8.83147600000000	1.51203000000000
H	-5.36129800000000	-8.34279100000000	-0.57674500000000
H	-4.87805500000000	-6.25786700000000	-1.89303700000000
H	-3.10636800000000	-4.67180000000000	-1.12193700000000
C	3.20681300000000	-7.04570600000000	1.21321300000000
C	4.34219800000000	-7.46894900000000	1.91869200000000
C	5.28249900000000	-6.52652800000000	2.37216700000000
C	5.08309000000000	-5.15927200000000	2.12317700000000
C	3.93980600000000	-4.72924700000000	1.42923400000000
H	2.49691800000000	-7.79437100000000	0.82564600000000
H	4.50350600000000	-8.54185300000000	2.10313900000000
H	6.17910400000000	-6.86370700000000	2.91443500000000
H	5.81890200000000	-4.41790400000000	2.46843700000000
H	3.78017000000000	-3.65569300000000	1.23173900000000
C	0.61017500000000	-7.34784000000000	-1.40173600000000
C	0.64767800000000	-8.24667200000000	-2.48060200000000
C	1.53063500000000	-8.02781500000000	-3.55095600000000
C	2.37171700000000	-6.90156800000000	-3.54636200000000
C	2.34454600000000	-6.00463200000000	-2.46833100000000
H	-0.10480300000000	-7.50681200000000	-0.57966100000000
H	-0.02334600000000	-9.11916100000000	-2.48681200000000
H	1.55752900000000	-8.73241000000000	-4.39581900000000
H	3.05436100000000	-6.71483700000000	-4.38866300000000
H	3.00494300000000	-5.12155800000000	-2.47756200000000
C	-1.19823900000000	-0.81966500000000	5.35458500000000
C	-2.28190700000000	-0.74206200000000	6.24231700000000
C	-2.27764700000000	0.20206700000000	7.28135400000000
C	-1.17561300000000	1.05704500000000	7.44483500000000
C	-0.08070300000000	0.97483200000000	6.56913900000000
H	-1.21648100000000	-1.55095900000000	4.53231600000000
H	-3.14300900000000	-1.41181500000000	6.10490300000000
H	-3.13959200000000	0.27357000000000	7.96140600000000
H	-1.16393200000000	1.79313300000000	8.26301400000000
H	0.78558600000000	1.63584400000000	6.72673300000000

C	2.66710300000000	-1.37583400000000	6.47158300000000
C	3.39646000000000	-2.41943600000000	7.05601400000000
C	3.78466200000000	-3.52715200000000	6.28011700000000
C	3.45400800000000	-3.58419900000000	4.91740000000000
C	2.73220800000000	-2.53466800000000	4.32462000000000
H	2.34865700000000	-0.51690500000000	7.08197100000000
H	3.65604400000000	-2.37597400000000	8.12480900000000
H	4.34819500000000	-4.35126700000000	6.74383000000000
H	3.75945700000000	-4.44735100000000	4.30843500000000
H	2.47361200000000	-2.56697900000000	3.25305400000000
C	4.51145800000000	4.30064400000000	3.04467100000000
C	5.11705400000000	5.48755900000000	3.47955800000000
C	5.18235600000000	5.77976500000000	4.85246700000000
C	4.63896300000000	4.88295800000000	5.78861300000000
C	4.04491400000000	3.68529000000000	5.35956900000000
H	4.42335300000000	4.08713000000000	1.96780200000000
H	5.51868000000000	6.19729600000000	2.74022200000000
H	5.65054200000000	6.71478600000000	5.19584200000000
H	4.68335800000000	5.11602200000000	6.86345200000000
H	3.62030000000000	2.98068600000000	6.09130500000000
C	4.81938200000000	-0.25167800000000	2.33696600000000
C	5.78137400000000	-1.27107500000000	2.42429700000000
C	6.46964100000000	-1.47913300000000	3.62881000000000
C	6.19222800000000	-0.67303500000000	4.74759700000000
C	5.23459900000000	0.34616700000000	4.66164200000000
H	4.25544500000000	-0.09273500000000	1.40437600000000
H	6.00756300000000	-1.90146500000000	1.54997200000000
H	7.23194900000000	-2.27076900000000	3.69239200000000
H	6.72636100000000	-0.84086400000000	5.69478500000000
H	5.01827300000000	0.96956000000000	5.54183700000000
C	-2.77217400000000	6.64635500000000	0.65841200000000
C	-4.04389200000000	7.23587800000000	0.71811000000000
C	-5.19289100000000	6.47135600000000	0.44055800000000
C	-5.07117300000000	5.11307900000000	0.10831700000000
C	-3.80031300000000	4.51877900000000	0.05073700000000
H	-1.87784400000000	7.24456800000000	0.88987000000000
H	-4.14048400000000	8.29878000000000	0.98738100000000
H	-6.18933800000000	6.93685600000000	0.49158400000000
H	-5.96954600000000	4.50965600000000	-0.09607600000000
H	-3.69732600000000	3.45060000000000	-0.19300200000000
C	0.74790000000000	6.46411100000000	1.19139600000000
C	1.55621500000000	7.02165800000000	2.19400200000000
C	1.65791400000000	6.39843000000000	3.44844800000000
C	0.95175500000000	5.20998400000000	3.69667300000000
C	0.16457200000000	4.63225700000000	2.68984400000000
H	0.66326200000000	6.95177600000000	0.21034500000000
H	2.11145600000000	7.94992400000000	1.99018300000000
H	2.29602100000000	6.83165400000000	4.23281500000000
H	1.02442400000000	4.72885200000000	4.68450200000000
H	-0.37995200000000	3.69532000000000	2.88244300000000
C	0.14836400000000	6.15001100000000	-4.27021400000000
C	0.08354600000000	6.47707400000000	-5.63304700000000
C	0.60552900000000	5.59642700000000	-6.59679900000000

C	1.18353000000000	4.38105600000000	-6.19475800000000
C	1.24681200000000	4.04659600000000	-4.83317700000000
H	-0.27171500000000	6.84479600000000	-3.52622100000000
H	-0.37739800000000	7.42635200000000	-5.94569100000000
H	0.55574800000000	5.85808100000000	-7.66455300000000
H	1.58859700000000	3.68516400000000	-6.94506000000000
H	1.69998300000000	3.09179100000000	-4.52107900000000
C	2.43683600000000	6.90392800000000	-1.83720600000000
C	3.54200800000000	7.65961600000000	-1.42276900000000
C	4.61186400000000	7.03834400000000	-0.75263600000000
C	4.56614000000000	5.66105900000000	-0.49155100000000
C	3.44958700000000	4.90679800000000	-0.88882300000000
H	1.61673800000000	7.40122500000000	-2.37554900000000
H	3.57625300000000	8.73906600000000	-1.63513100000000
H	5.48645400000000	7.63190600000000	-0.44475300000000
H	5.40973000000000	5.15985400000000	0.00661000000000
H	3.40950200000000	3.82730000000000	-0.67474800000000
C	-6.22732800000000	0.65999000000000	-4.58792500000000
C	-7.54109900000000	0.23685100000000	-4.84641000000000
C	-8.07807800000000	-0.86577600000000	-4.15799400000000
C	-7.29899300000000	-1.55307300000000	-3.21195000000000
C	-5.98520900000000	-1.13635600000000	-2.95110400000000
H	-5.81468900000000	1.53198200000000	-5.11902800000000
H	-8.15172800000000	0.77418700000000	-5.58813300000000
H	-9.11205500000000	-1.18627600000000	-4.35662200000000
H	-7.71721400000000	-2.40474700000000	-2.65393400000000
H	-5.38118400000000	-1.66509400000000	-2.19582500000000
C	-2.59839800000000	2.60492700000000	-4.70348300000000
C	-2.45351300000000	3.97178200000000	-4.98440200000000
C	-3.24878300000000	4.91963000000000	-4.31988100000000
C	-4.19589400000000	4.49735600000000	-3.37046500000000
C	-4.34574600000000	3.13194600000000	-3.08776500000000
H	-1.96537400000000	1.86654500000000	-5.21789800000000
H	-1.71097700000000	4.29696100000000	-5.72685600000000
H	-3.13350400000000	5.99030000000000	-4.54848400000000
H	-4.82039200000000	5.23272000000000	-2.84153400000000
H	-5.09136300000000	2.81113300000000	-2.34111000000000
C	-3.36810100000000	-3.48605700000000	-4.47925000000000
C	-3.77082500000000	-4.83182100000000	-4.46904600000000
C	-2.85041900000000	-5.84181700000000	-4.14496000000000
C	-1.52874500000000	-5.50480000000000	-3.80574700000000
C	-1.12571100000000	-4.16232700000000	-3.80184000000000
H	-4.09341100000000	-2.69719500000000	-4.73058700000000
H	-4.81044600000000	-5.08940600000000	-4.72445700000000
H	-3.16459100000000	-6.89651000000000	-4.14316400000000
H	-0.80914000000000	-6.28834200000000	-3.53056800000000
H	-0.09555300000000	-3.90785300000000	-3.50637300000000
C	-0.47987300000000	-2.20624800000000	-6.72535500000000
C	0.30800100000000	-2.01904200000000	-7.87279000000000
C	1.10723100000000	-0.87184900000000	-8.00260400000000
C	1.12150200000000	0.09169400000000	-6.97937500000000
C	0.34811900000000	-0.09412600000000	-5.82547800000000
H	-1.10541100000000	-3.10700300000000	-6.62812000000000

H	0.29371600000000	-2.77440300000000	-8.67319200000000
H	1.72300600000000	-0.72974300000000	-8.90364000000000
H	1.75175700000000	0.98907100000000	-7.07099800000000
H	0.38241400000000	0.64758600000000	-5.01080200000000
C	-4.50010200000000	3.51888200000000	3.13937800000000
C	-4.16901100000000	4.77272600000000	3.67824100000000
C	-3.09850600000000	4.89395900000000	4.57792100000000
C	-2.35069700000000	3.75768100000000	4.93274000000000
C	-2.65775600000000	2.50837200000000	4.37665100000000
H	-5.33821700000000	3.41704400000000	2.43438700000000
H	-4.74931400000000	5.66023700000000	3.38409900000000
H	-2.84030400000000	5.87725900000000	4.99916800000000
H	-1.51373200000000	3.84445700000000	5.64267700000000
H	-2.05890700000000	1.62469800000000	4.64013100000000
C	-5.58389200000000	0.63304900000000	5.27905000000000
C	-6.28975200000000	-0.03655200000000	6.29023800000000
C	-6.53360200000000	-1.41617200000000	6.18882700000000
C	-6.05837200000000	-2.13170700000000	5.07604600000000
C	-5.33096500000000	-1.47300500000000	4.07529800000000
H	-5.40489200000000	1.71570300000000	5.35747400000000
H	-6.66227800000000	0.52677100000000	7.15936200000000
H	-7.09699700000000	-1.93579400000000	6.97865400000000
H	-6.25568100000000	-3.21110100000000	4.98780700000000
H	-4.93658600000000	-2.04124000000000	3.21852600000000
C	-8.10179900000000	3.11657700000000	0.65984200000000
C	-8.44885700000000	4.08680600000000	-0.29530500000000
C	-8.20159300000000	3.85017300000000	-1.65928300000000
C	-7.61416100000000	2.63905100000000	-2.06644400000000
C	-7.26970100000000	1.66725900000000	-1.11390000000000
H	-8.30236300000000	3.29717400000000	1.72843600000000
H	-8.92363000000000	5.02681300000000	0.02553800000000
H	-8.48030400000000	4.60630400000000	-2.40912500000000
H	-7.43096900000000	2.43998700000000	-3.13399400000000
H	-6.83083600000000	0.71196000000000	-1.44515400000000
C	-8.44343000000000	-1.40116300000000	0.37222700000000
C	-8.60305700000000	-2.69332100000000	-0.15010800000000
C	-7.48656400000000	-3.53225500000000	-0.32503900000000
C	-6.20725800000000	-3.06193500000000	0.00991600000000
C	-6.04769700000000	-1.76443200000000	0.52528700000000
H	-9.32992500000000	-0.76214800000000	0.51800700000000
H	-9.60966700000000	-3.05333500000000	-0.41298400000000
H	-7.61652500000000	-4.55270600000000	-0.71750000000000
H	-5.32163900000000	-3.70305700000000	-0.12679000000000
H	-5.03315300000000	-1.41521000000000	0.77281700000000
C	5.08762100000000	-2.55133500000000	-4.20801700000000
C	4.97911700000000	-3.59468000000000	-5.14039500000000
C	3.71318300000000	-4.04177600000000	-5.55743100000000
C	2.55148300000000	-3.45958400000000	-5.02505500000000
C	2.65634500000000	-2.42950800000000	-4.07724900000000
H	6.08221200000000	-2.18222300000000	-3.90985100000000
H	5.89062700000000	-4.05140800000000	-5.55512200000000
H	3.63265300000000	-4.84670000000000	-6.30417800000000
H	1.55925600000000	-3.80832200000000	-5.34646500000000

H	1.74526500000000	-1.97723300000000	-3.64933700000000
C	4.13505200000000	0.84182100000000	-4.99352500000000
C	4.32330500000000	1.99607000000000	-5.77216600000000
C	4.66028700000000	3.21664700000000	-5.16532400000000
C	4.80725800000000	3.28423900000000	-3.76897100000000
C	4.61727100000000	2.13752100000000	-2.98602200000000
H	3.87803800000000	-0.11076800000000	-5.48031700000000
H	4.22047600000000	1.93509000000000	-6.86697400000000
H	4.80745300000000	4.11757800000000	-5.77971300000000
H	5.07115100000000	4.23487800000000	-3.28187000000000
H	4.74549700000000	2.19427500000000	-1.89469100000000
C	8.95135000000000	-1.22219000000000	0.01537200000000
C	9.50504400000000	-2.16155400000000	0.90030300000000
C	8.96820600000000	-3.45618100000000	0.98917300000000
C	7.87630600000000	-3.81247400000000	0.17869200000000
C	7.31913800000000	-2.87635300000000	-0.70558700000000
H	9.37804900000000	-0.20895700000000	-0.03568100000000
H	10.36386700000000	-1.87593000000000	1.52682700000000
H	9.40771300000000	-4.19070900000000	1.68135400000000
H	7.45375800000000	-4.82761200000000	0.23126400000000
H	6.45871500000000	-3.16478500000000	-1.33023100000000
C	8.00890100000000	2.27065200000000	-2.00311100000000
C	8.22863200000000	3.55356900000000	-1.47249700000000
C	7.87535500000000	3.83279800000000	-0.14279400000000
C	7.30096400000000	2.82808700000000	0.65820800000000
C	7.08807200000000	1.54720300000000	0.12880400000000
H	8.27281800000000	2.05578200000000	-3.05103000000000
H	8.67922900000000	4.33673500000000	-2.10106600000000
H	8.05889500000000	4.83459900000000	0.27631300000000
H	7.02866600000000	3.03867300000000	1.70461400000000
H	6.65584900000000	0.76718700000000	0.77278900000000
N	-0.43992800000000	5.18205000000000	-1.33125300000000
H	-1.22502900000000	5.31006200000000	-1.98778900000000
N	5.42837800000000	-0.69143900000000	-1.57504000000000
H	5.23726800000000	-0.86314700000000	-0.58147700000000
N	2.17617000000000	1.36546800000000	4.62677300000000
H	1.48466500000000	2.11966500000000	4.76866700000000
N	-5.29910700000000	0.98962700000000	1.55887200000000
H	-4.83924800000000	1.00061200000000	0.63440300000000
N	0.19853800000000	-5.51725500000000	1.04259100000000
H	0.27944800000000	-6.38893600000000	1.58263900000000
N	-2.81922800000000	-0.43415800000000	-4.49987600000000
H	-3.19636800000000	-0.44022200000000	-5.45692800000000

Table S22: Cartesian coordinates for $[Ag_{10}H_8(dppa)_6]^{2+}$ via $\mathbf{4c}^{2+}$.

P	-3.49872500000000	-1.11113900000000	4.33709700000000
Ag	-2.97954700000000	-0.13047500000000	2.18731000000000
Ag	-1.02696800000000	1.59910200000000	0.99783900000000
P	-0.67013200000000	4.05662300000000	1.44260200000000
P	-2.15863500000000	4.42567100000000	-1.23299000000000
Ag	-2.52867100000000	1.98108100000000	-1.41206200000000
P	-4.83401900000000	1.86564400000000	-2.36166400000000
P	-4.93571300000000	-1.04191100000000	-1.59922500000000
Ag	-2.58851100000000	-0.74576400000000	-0.62968200000000
Ag	0.94831800000000	-2.62742000000000	-0.57404800000000
P	-0.23056300000000	-4.20995700000000	-2.11990400000000
P	-0.34745700000000	-1.76995200000000	-3.94815700000000
Ag	0.71387600000000	-0.27387800000000	-2.28740900000000
Ag	3.30777700000000	-0.90960400000000	-0.61998900000000
P	5.56582700000000	-1.90349400000000	-1.09833100000000
P	4.15576100000000	-2.76457900000000	1.33274700000000
Ag	-0.73440100000000	-1.85166300000000	1.57256700000000
P	-0.91141200000000	-2.57008200000000	3.99535900000000
Ag	2.12785700000000	1.85476500000000	-1.20085400000000
P	4.03977800000000	3.34990100000000	-0.90059900000000
P	5.26879900000000	2.58105700000000	1.81576900000000
Ag	1.34787000000000	0.09994000000000	1.01614600000000
H	-2.88593700000000	1.46681400000000	1.40880300000000
H	-2.46148000000000	-1.78262100000000	0.87575500000000
H	-1.35844300000000	0.63250900000000	-1.04130800000000
H	0.55291300000000	-3.00708700000000	1.12271000000000
H	-0.13693700000000	0.19116300000000	1.96045000000000
H	2.04225000000000	-1.73215200000000	-1.75824500000000
H	2.95379800000000	0.68286100000000	0.33116500000000
H	0.97745700000000	1.49952200000000	-2.53562000000000
C	-6.26763000000000	-0.99410400000000	-0.32920500000000
C	-5.38783100000000	-2.50180600000000	-2.62752900000000
C	-5.26245400000000	2.67301900000000	-3.95008900000000
C	-6.02888900000000	2.49858200000000	-1.10451100000000
C	0.82135600000000	5.07037100000000	1.84984400000000
C	-1.76930800000000	4.49053700000000	2.86876400000000
C	-3.72277000000000	5.38485700000000	-1.08233000000000
C	-1.31516600000000	5.09250700000000	-2.72641900000000
C	6.83085900000000	3.40149000000000	2.37449500000000
C	4.18524000000000	2.84206600000000	3.30480300000000
C	4.04108900000000	5.03200500000000	-1.66019700000000
C	5.48338300000000	2.54737500000000	-1.71407300000000
C	-1.62941200000000	-5.15505200000000	-1.40758900000000
C	0.76093400000000	-5.46745200000000	-3.02658200000000
C	0.93663800000000	-2.18600400000000	-5.21500100000000
C	-1.69342100000000	-1.23445900000000	-5.09348800000000
C	7.25200700000000	-1.18452300000000	-0.90795000000000
C	5.72172600000000	-2.98555600000000	-2.57645900000000
C	3.47784700000000	-4.45635500000000	1.52559700000000
C	4.99177700000000	-2.39385800000000	2.93233100000000
C	0.61326800000000	-2.46918300000000	5.01245700000000

C	-1.45254100000000	-4.32645600000000	4.15901900000000
C	-4.63091700000000	-2.56605600000000	4.39046500000000
C	-4.14185300000000	0.03562900000000	5.61177700000000
C	-6.40634500000000	-3.40247200000000	-2.25319200000000
C	-6.65856400000000	-4.54147500000000	-3.03481400000000
C	-5.90938600000000	-4.78542800000000	-4.19630000000000
C	-4.90271700000000	-3.88299500000000	-4.57897900000000
C	-4.63455100000000	-2.75287200000000	-3.79445500000000
H	-7.00612400000000	-3.21385800000000	-1.35028300000000
H	-7.45378300000000	-5.24055700000000	-2.73460100000000
H	-6.11345000000000	-5.67808000000000	-4.80665600000000
H	-4.31779900000000	-4.05696600000000	-5.49530900000000
H	-3.82923900000000	-2.06488800000000	-4.09002500000000
C	-6.01441500000000	-1.51897300000000	0.95283400000000
C	-7.01913000000000	-1.49681600000000	1.93482300000000
C	-8.27156700000000	-0.93340600000000	1.64430000000000
C	-8.52737900000000	-0.40900300000000	0.36516800000000
C	-7.53333800000000	-0.44525900000000	-0.62163500000000
H	-5.02758200000000	-1.95094700000000	1.18143100000000
H	-6.81699600000000	-1.92449600000000	2.92777900000000
H	-9.05482400000000	-0.90596600000000	2.41723900000000
H	-9.50738400000000	0.03578100000000	0.13535400000000
H	-7.72116600000000	-0.02631900000000	-1.62088200000000
C	-4.33274000000000	3.57045400000000	-4.51432600000000
C	-4.59480500000000	4.18544400000000	-5.74798800000000
C	-5.78508500000000	3.89767800000000	-6.43565500000000
C	-6.70967700000000	2.99103000000000	-5.88858000000000
C	-6.45468700000000	2.38061200000000	-4.65058500000000
H	-3.37849600000000	3.76250700000000	-4.00221900000000
H	-3.85568300000000	4.87856400000000	-6.17786500000000
H	-5.99061000000000	4.37358900000000	-7.40646400000000
H	-7.63934900000000	2.75830800000000	-6.42978800000000
H	-7.18120800000000	1.66657700000000	-4.23316100000000
C	-7.23891900000000	3.14889200000000	-1.42041200000000
C	-8.12313900000000	3.51941000000000	-0.39505400000000
C	-7.80916900000000	3.24814300000000	0.94759800000000
C	-6.59329600000000	2.62458600000000	1.26852200000000
C	-5.70374200000000	2.26150800000000	0.24829800000000
H	-7.49411100000000	3.37885300000000	-2.46510700000000
H	-9.06480200000000	4.02982900000000	-0.64869700000000
H	-8.51139900000000	3.53730700000000	1.74451800000000
H	-6.32214400000000	2.42222700000000	2.31647900000000
H	-4.74624300000000	1.78651200000000	0.51985900000000
C	-4.38311100000000	5.98407400000000	-2.17680400000000
C	-5.63087700000000	6.60242600000000	-1.99896200000000
C	-6.23321800000000	6.63010500000000	-0.73225900000000
C	-5.58483600000000	6.03074400000000	0.36012300000000
C	-4.34356300000000	5.40506900000000	0.18769900000000
H	-3.92697600000000	5.98043800000000	-3.17588000000000
H	-6.13102000000000	7.06922700000000	-2.86104600000000
H	-7.21078000000000	7.11655500000000	-0.59574500000000
H	-6.05247600000000	6.03705800000000	1.35588700000000
H	-3.85635100000000	4.92691500000000	1.05075500000000

C	-0.66170200000000	4.16688300000000	-3.56982500000000
C	-0.03383200000000	4.60069200000000	-4.74807300000000
C	-0.05559500000000	5.96172700000000	-5.09361300000000
C	-0.68209100000000	6.89332300000000	-4.24566700000000
C	-1.30407100000000	6.46436100000000	-3.06333400000000
H	-0.63040000000000	3.09869900000000	-3.29508100000000
H	0.47289400000000	3.86934900000000	-5.39567900000000
H	0.42589300000000	6.30198000000000	-6.02315600000000
H	-0.68838100000000	7.96206000000000	-4.50919600000000
H	-1.80228000000000	7.20058300000000	-2.41319100000000
C	-2.20264400000000	3.47729500000000	3.74662400000000
C	-3.06028300000000	3.78202100000000	4.81633300000000
C	-3.49644300000000	5.10098900000000	5.01116800000000
C	-3.06213700000000	6.12094600000000	4.14536100000000
C	-2.19712300000000	5.81923400000000	3.08432400000000
H	-1.88842100000000	2.43504100000000	3.58039700000000
H	-3.39492300000000	2.98122800000000	5.49121000000000
H	-4.17652500000000	5.33765900000000	5.84384600000000
H	-3.39591700000000	7.15825200000000	4.30040200000000
H	-1.85654700000000	6.63065000000000	2.42150700000000
C	1.21786400000000	5.26380100000000	3.19088200000000
C	2.35173200000000	6.03145400000000	3.49234800000000
C	3.08610400000000	6.64250900000000	2.46242800000000
C	2.68563600000000	6.47151300000000	1.12593700000000
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H	3.23898000000000	6.96135800000000	0.31103100000000
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C	2.48251100000000	2.93138200000000	5.57113100000000
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C	4.65689500000000	3.33614500000000	4.54136800000000
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H	1.82522100000000	2.95927400000000	6.45362400000000
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H	5.69427100000000	3.69171600000000	4.63232500000000
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C	8.96203200000000	3.16761400000000	3.55131700000000
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C	8.38775400000000	5.27869600000000	2.49275200000000
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C	5.08774500000000	7.19733200000000	-2.05837300000000
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H	-5.43042400000000	-0.02017300000000	-3.67181900000000

S.8. References

[S1] Fort, K. L.; Dyachenko, A.; Potel, C. M.; Corradini, E.; Marino, F.; Barendregt, A.; Makarov, A. A.; Scheltema, R. A.; Heck, A. J. R., *Anal. Chem.* **2016**, *88*, 2303-2310.