Electronic Supporting Information

Water-Soluble Silver Nanoparticles Stabilized by Amino Acid-Derived *N*-Heterocyclic Carbenes: Synthesis, Properties and Theoretical Study of Nucleation Process

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Figure S14. Energy profile of the stepwise formation of NP for the ligand $(NHC^{H})^{2-}$.

Figure S15. Optimized structures of $[Ag_{20}(NHC^{Me})]^{2-}$ with carbene coordinated to a silver atom located on (a) face; (b) vertex; and (c) edge.

Figure S16. Optimized structures of $[Ag_{20}(NHC^{iPr})]^{2-}$ with carbene coordinated to a silver atom located on (a) face; (b) vertex; and (c) edge.

Figure S17. Comparison of BDE energies (kcal/mol) of the Ag-C bond in calculated compounds $[Ag_n(NHC^{R})]^{2-}$ (n = 1, 2, 30) for R = H, Me, and ^{i}Pr.

Table S1. BDE energies (kcal/mol) of the Ag-C bond in selected NHC-silver complexes and in calculated compounds $[Ag_n(NHC^{R})]^{2-}$ (n = 1, 2).

Table S2. Selected structural and energetic data of $[Ag(NHC^{R})]^{n-}$ and their corresponding $[Ag(\kappa^1\textit{O}\text{-}NHC^{R})]^{n-}$ isomers (n = 1, 2. R = H, Me, and ^{i}Pr).

Table S3. Selected local and integrated topological properties of the electron density at the Ag-X (X being Ag and C) for Ag_n clusters and $[Ag_n(NHC^{H})]^{2-}$ complexes (n = 3 or 4).[a]

Table S4. Selected structural data and relative energy data of $[Ag_{20}(NHC^{R})]^{2-}$ (R = H, Me, and ^{i}Pr) for the three different coordination types.

Table S5. Selected local and integrated topological properties of the electron density at the Ag-X (X being Ag and C) for $[Ag_{20}(NHC^{R})]^{2-}$ complexes (R = Me, ^{i}Pr).[a]

Table S6. Selected local and integrated topological properties of the electron density at the Ag-X (X being Ag and C) for $[Ag_{30}(NHC^{R})]^{2-}$ complexes (R = H, Me, ^{i}Pr).[a]

Table S7. Coordinates of the optimized compounds.

Figure S1. Dynamic light scattering (DLS) analysis of Ag(NHC^{H})-NPs (**3a**).

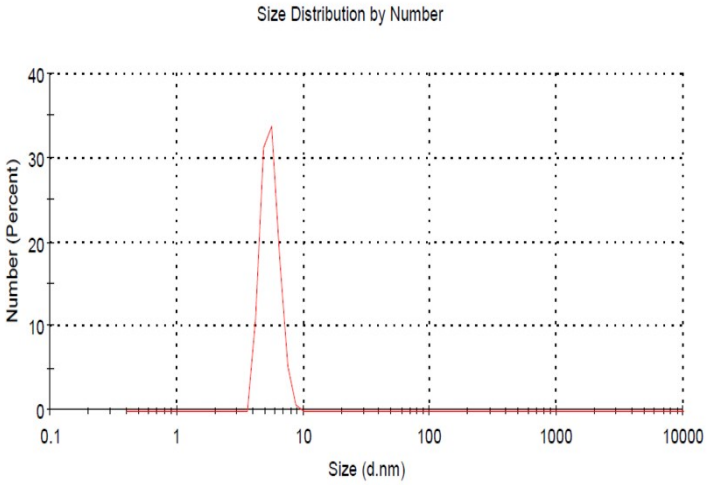


Figure S2. Transmission electron microscopy (TEM) images and particle size distribution analysis of Ag(NHC^{H})-NPs (**3a**), performed using ImageJ software.

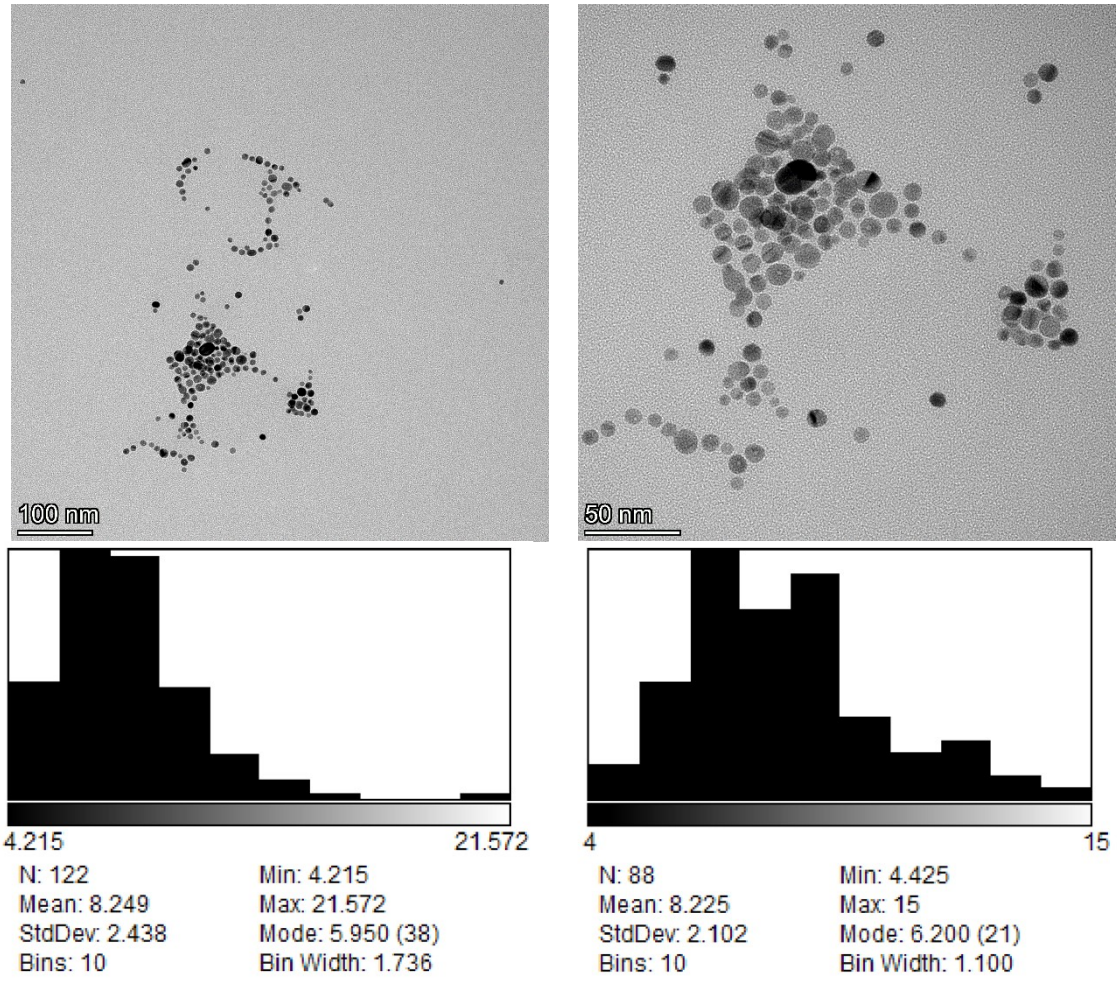


Figure S3. ATR-IR spectrum of Ag(NHC^H)-NPs (**3a**).

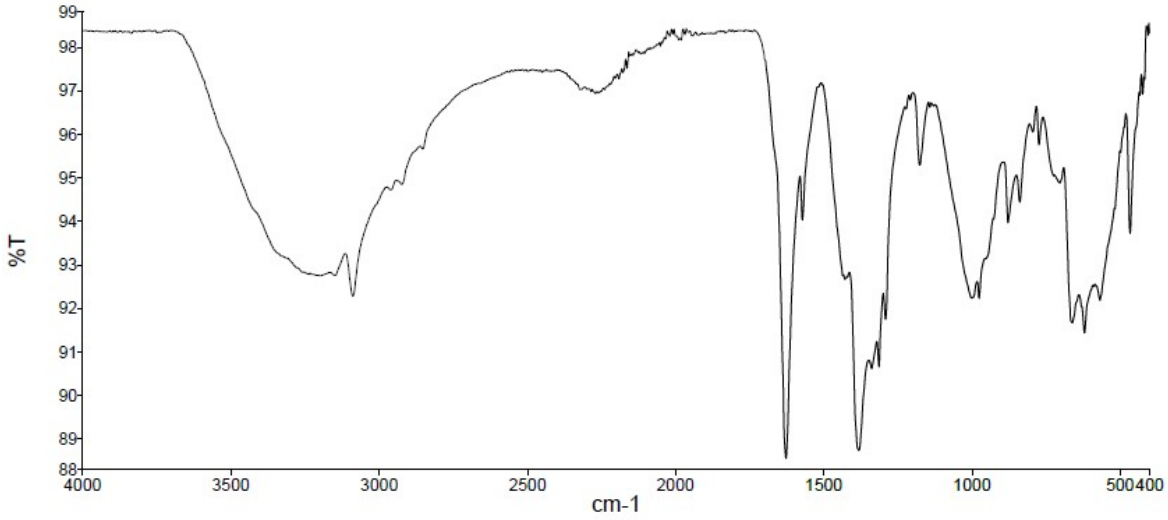


Figure S4. DLS analysis of non-stabilized AgNPs.

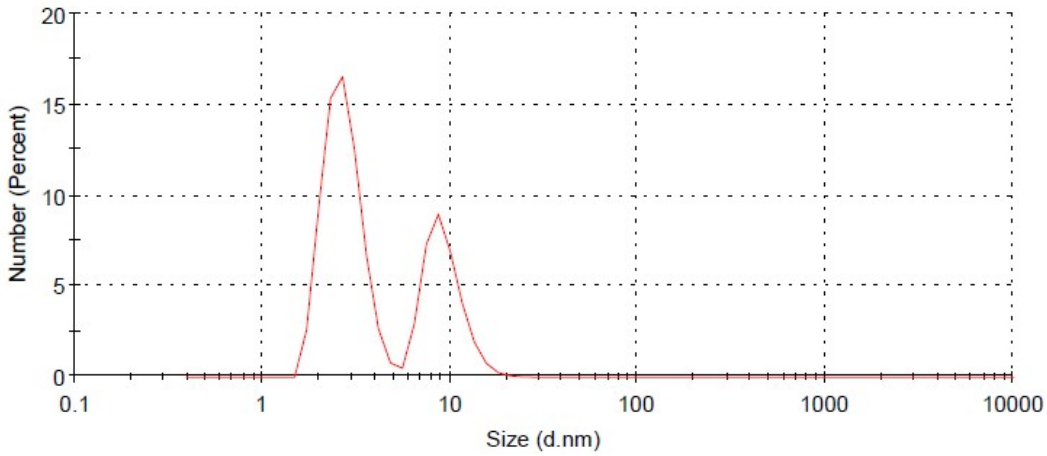
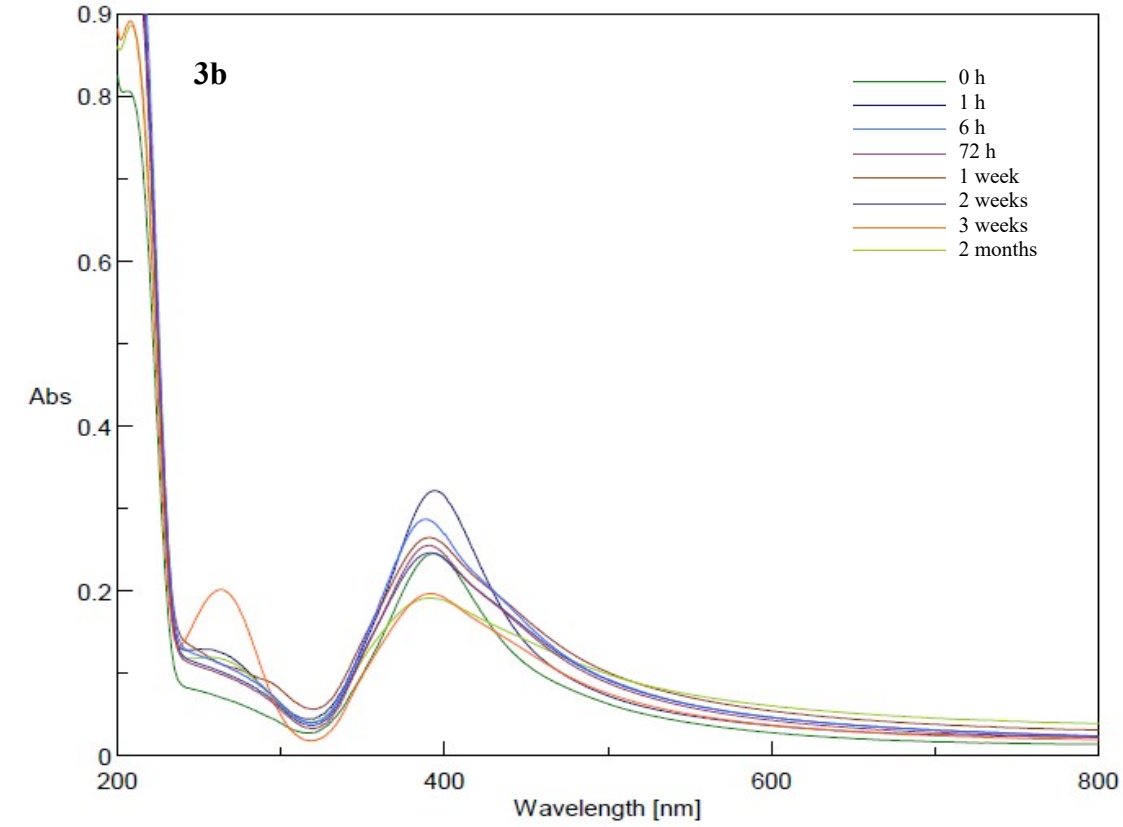
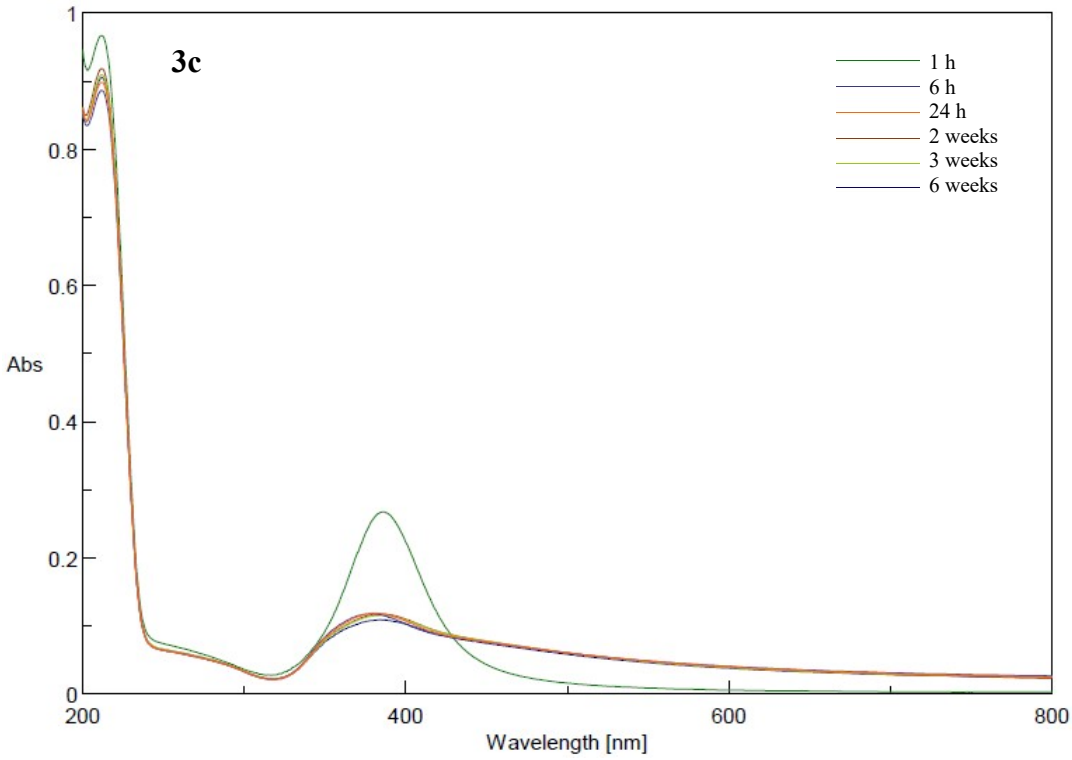


Figure S5. UV-vis spectrum of Ag(NHC^{R})-NPs (R = Me, **3b**; ^{i}Pr, **3c** and ^{i}Bu, **3d**) over time.





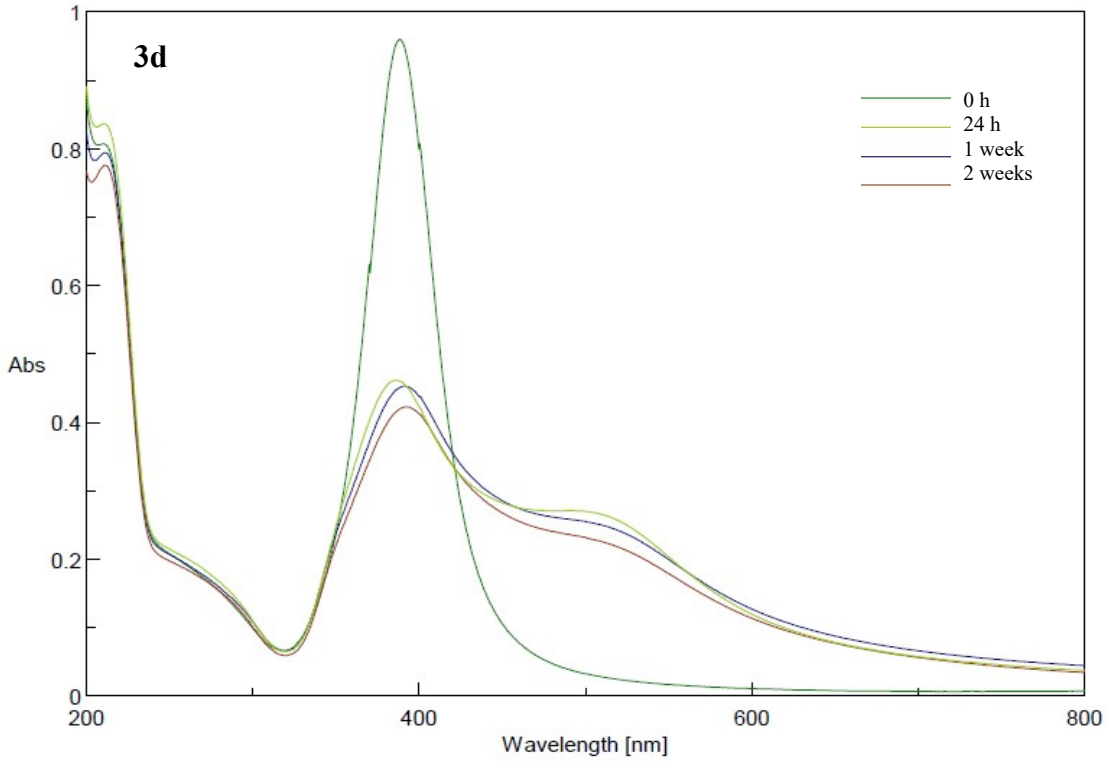

3d
0 h
24 h
1 week
2 weeks
Abs
Wavelength [nm]
0
0.2
0.4
0.6
0.8
1
200
400
600
800

Figure S6. DLS analysis, TEM images and particle size distribution analysis of Ag(NHC^{iPr})-NPs (**3c**).

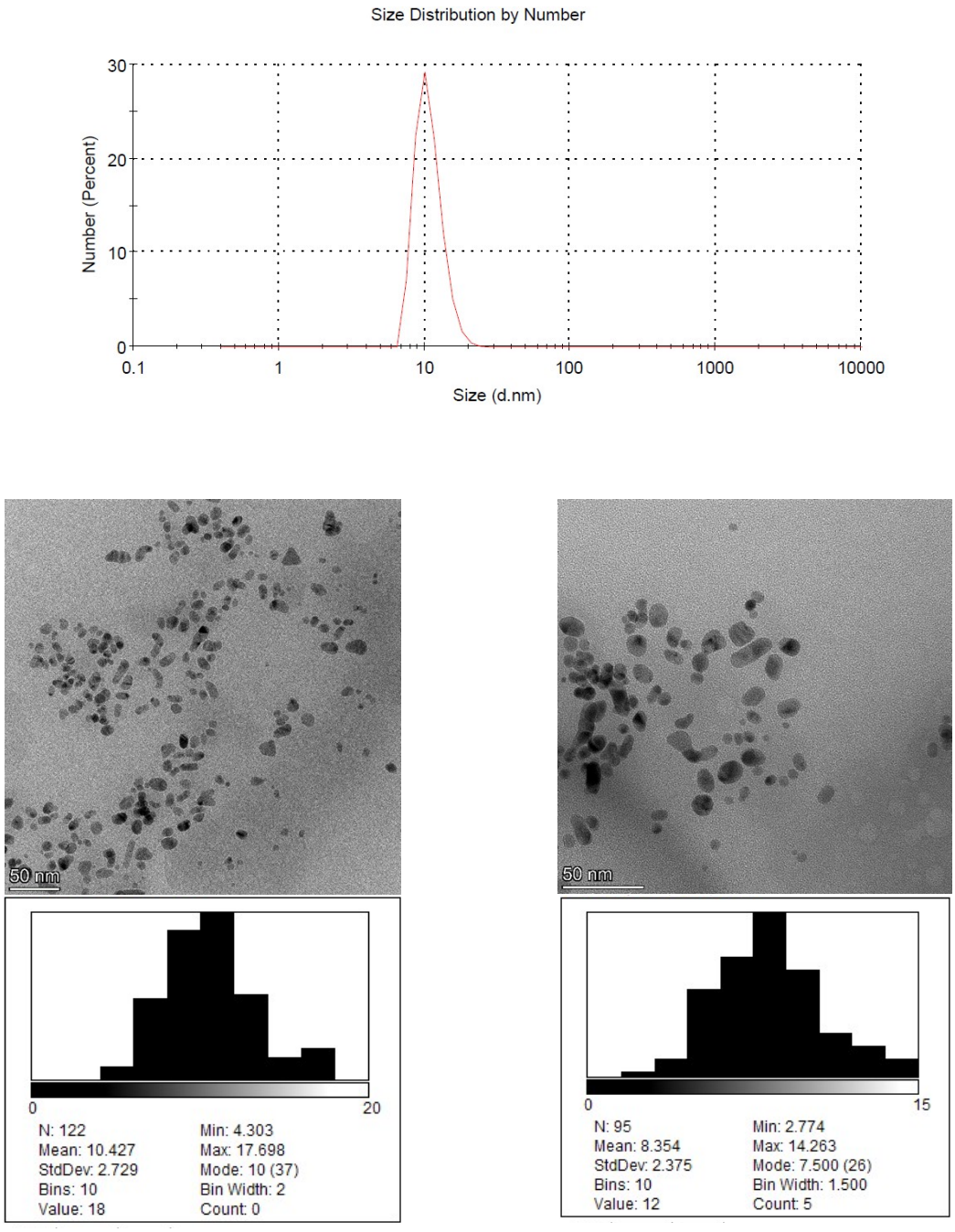


Figure S7. TEM images and particle size distribution analysis of Ag(NHC^{Me})-NPs (**3b**) and Ag(NHC^{iBu})-NPs (**3d**).

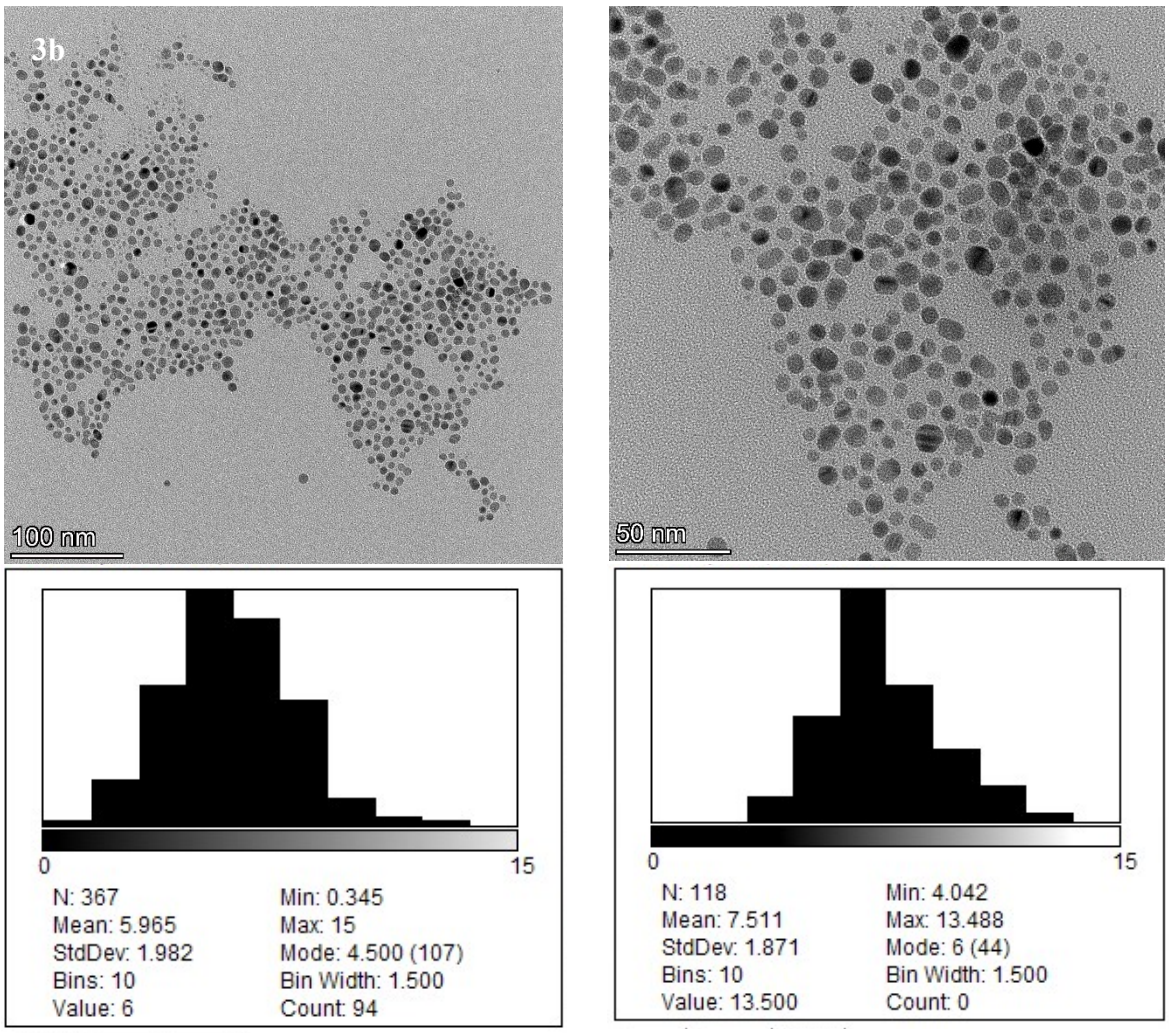
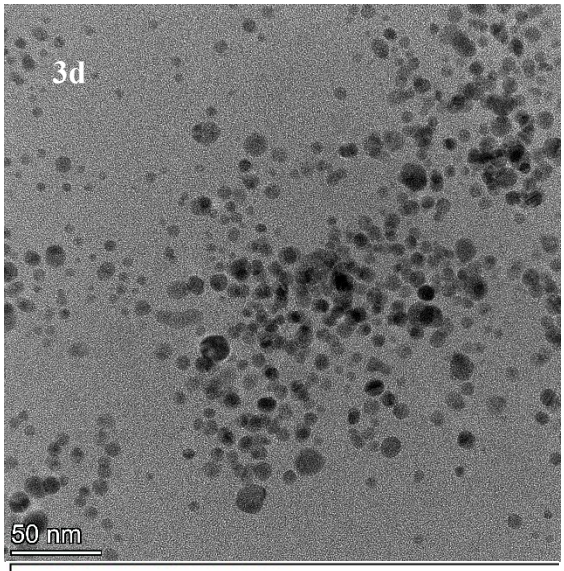
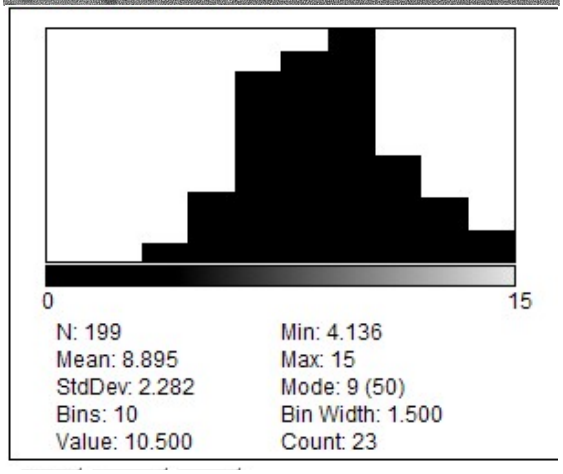
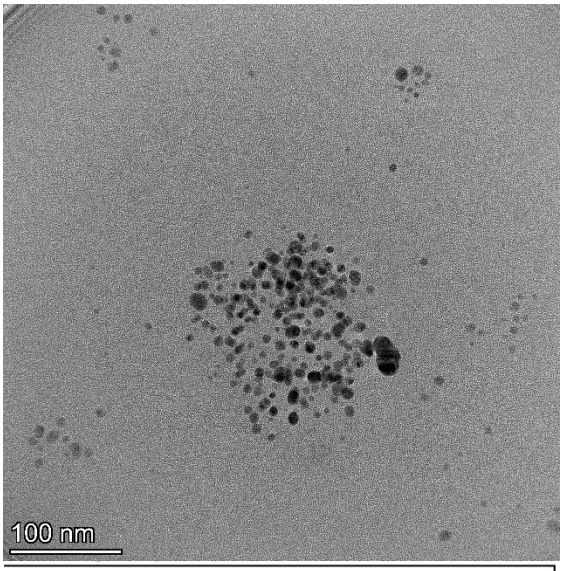


Figure S7 (cont.). TEM images and particle size distribution analysis of Ag(NHC^{Me})-NPs (**3b**) and Ag(NHC^{iBu})-NPs (**3d**).







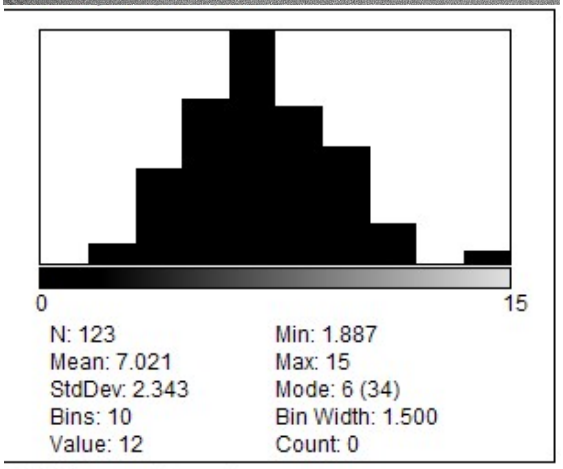


Figure S8. Catalytic activity of Ag(NHC^{H})-NPs (**3a**) in the reduction of 4-NP. UV−vis spectra showing the decrease in 4-NP absorption with the concomitant increase in the 4-AP absorption band.

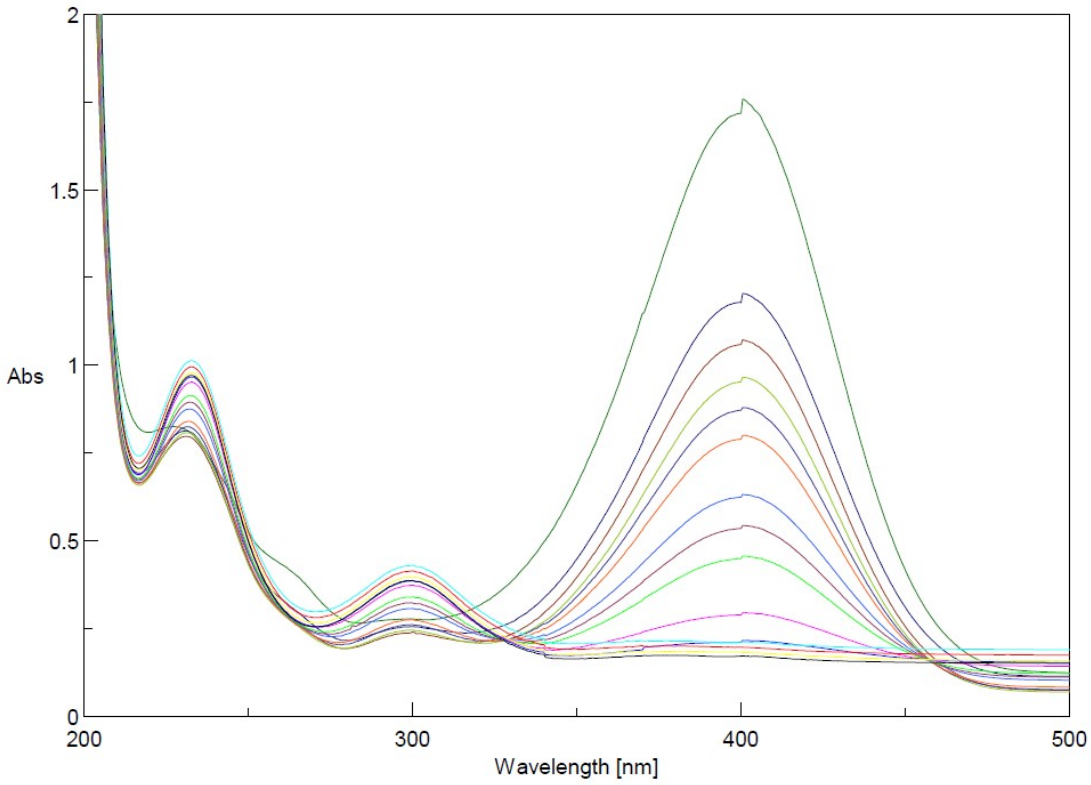


Figure S9. Kinetic profile of H_2 evolution from $NaBH_4$ hydrolysis catalyzed by AgNP **3a** in basic aqueous medium.

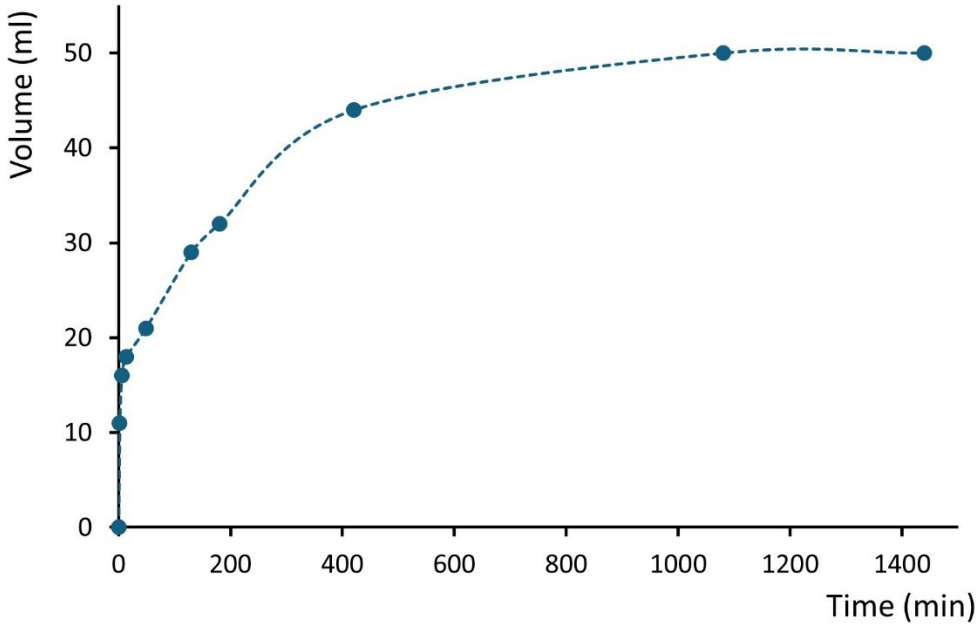


Figure S10. Optimized structures of $[Ag(NHC^R)]^-$ for R = H, Me, and ^{i}Pr.

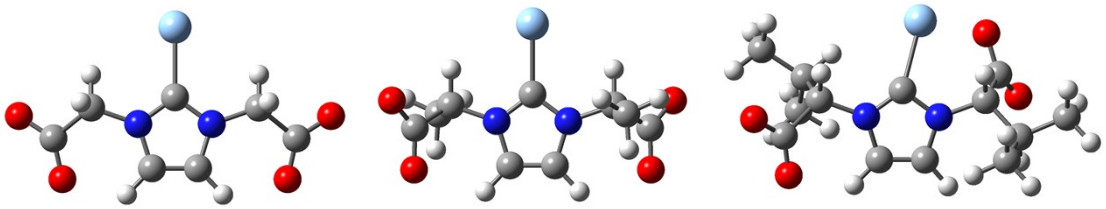


Figure S11. Simplified MO diagram of the $[Ag(NHC^{H})]^{2-}$ species.

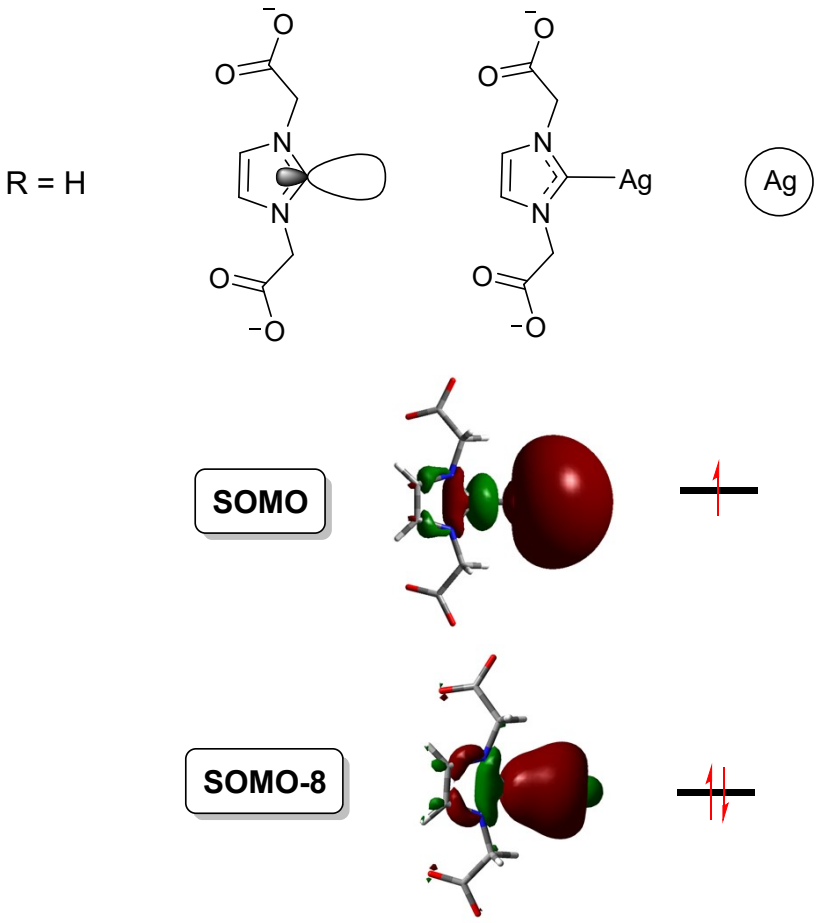


Figure S12. Simplified MO diagram of the $[Ag_2(NHC^H)]^{2-}$ species.

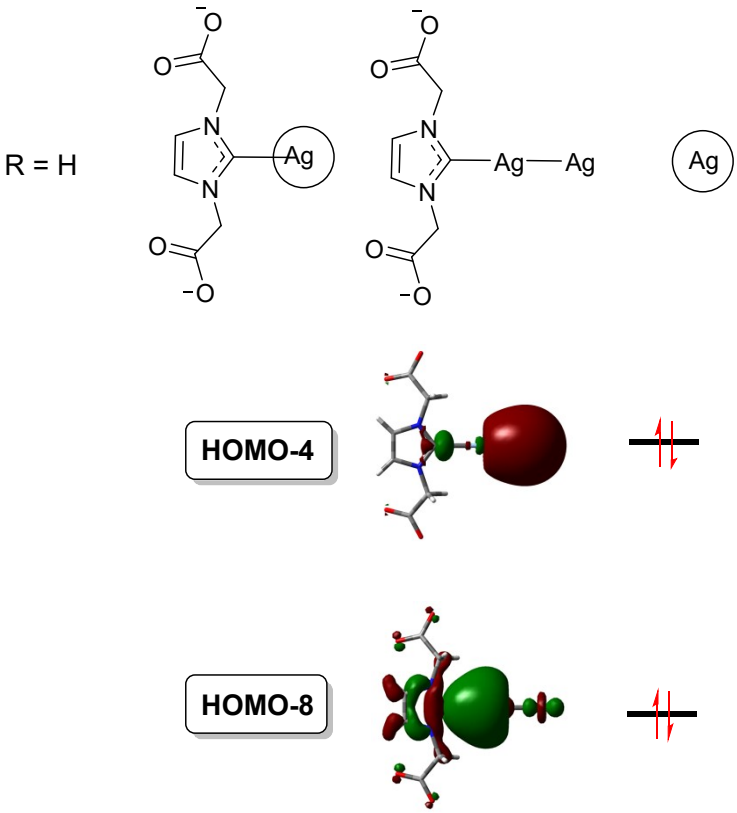
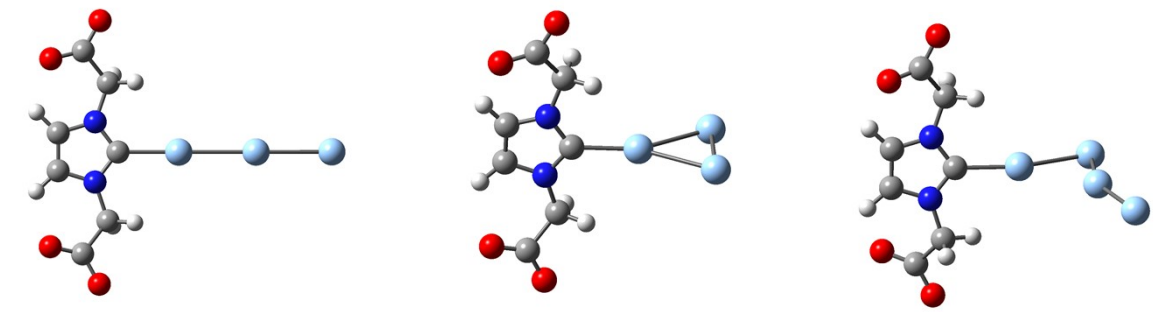


Figure S13. Optimized structures of $[Ag_n(NHC^H)]^{2-}$ (n = 3, 4).



$[Ag_3(NHC^H)]^{2-}$ (linear) $[Ag_3(NHC^H)]^{2-}$ (triangular) $[Ag_4(NHC^H)]^{2-}$

Figure S14. Energy profile of the stepwise formation of NP for the ligand $(NHC^{H})^{2-}$.

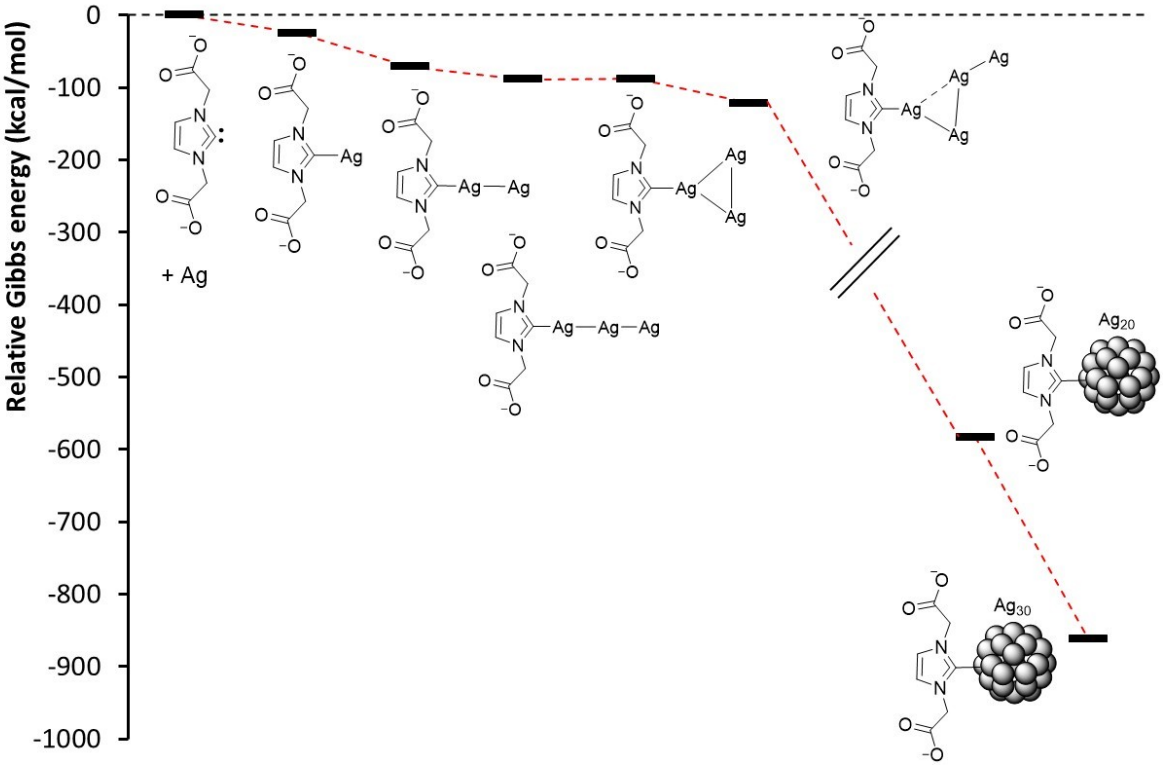
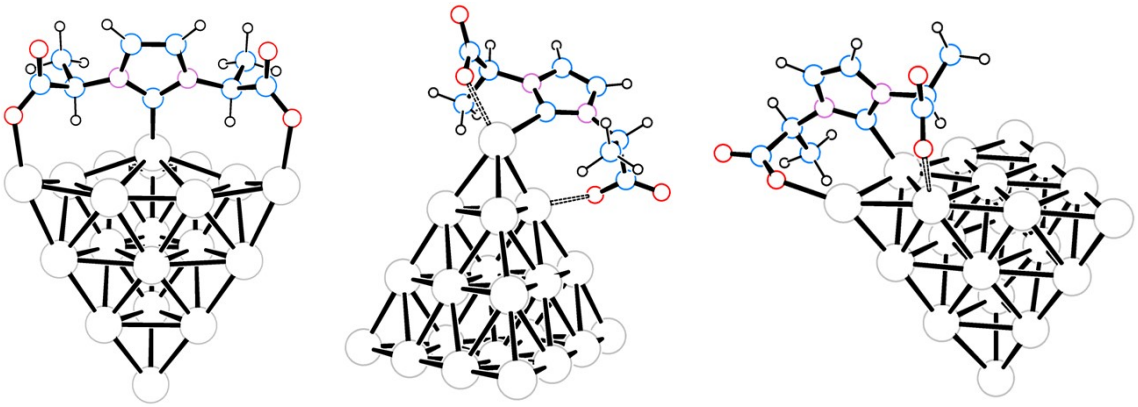
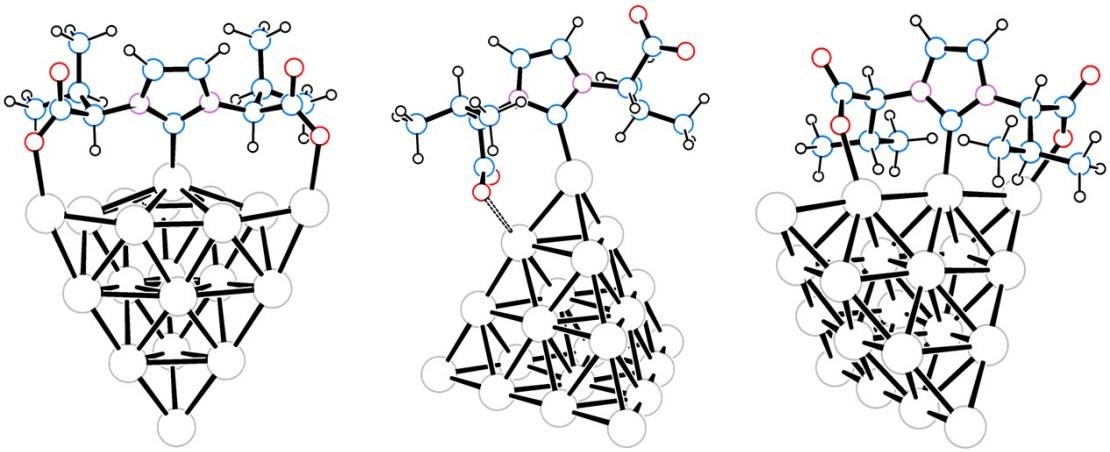


Figure S15. Optimized structures of $[Ag_{20}(NHC^{Me})]^{2-}$ with the carbene ligand coordinated to a silver atom situated at face (F), vertex (V) and edge (E).



(F) **(V)** **(E)**

Figure S16. Optimized structures of $[Ag_{20}(NHC^{iPr})]^{2-}$ with the carbene ligand coordinated to a silver atom situated face (F), vertex (V) and edge (E).



(F) **(V)** **(E)**

Figure S17. Comparison of BDE energies (kcal/mol) of the Ag-C bond in calculated compounds $[Ag_n(NHC^R)]^{2-}$ (n = 1, 2, 30) for R = H, Me, and ^{i}Pr.

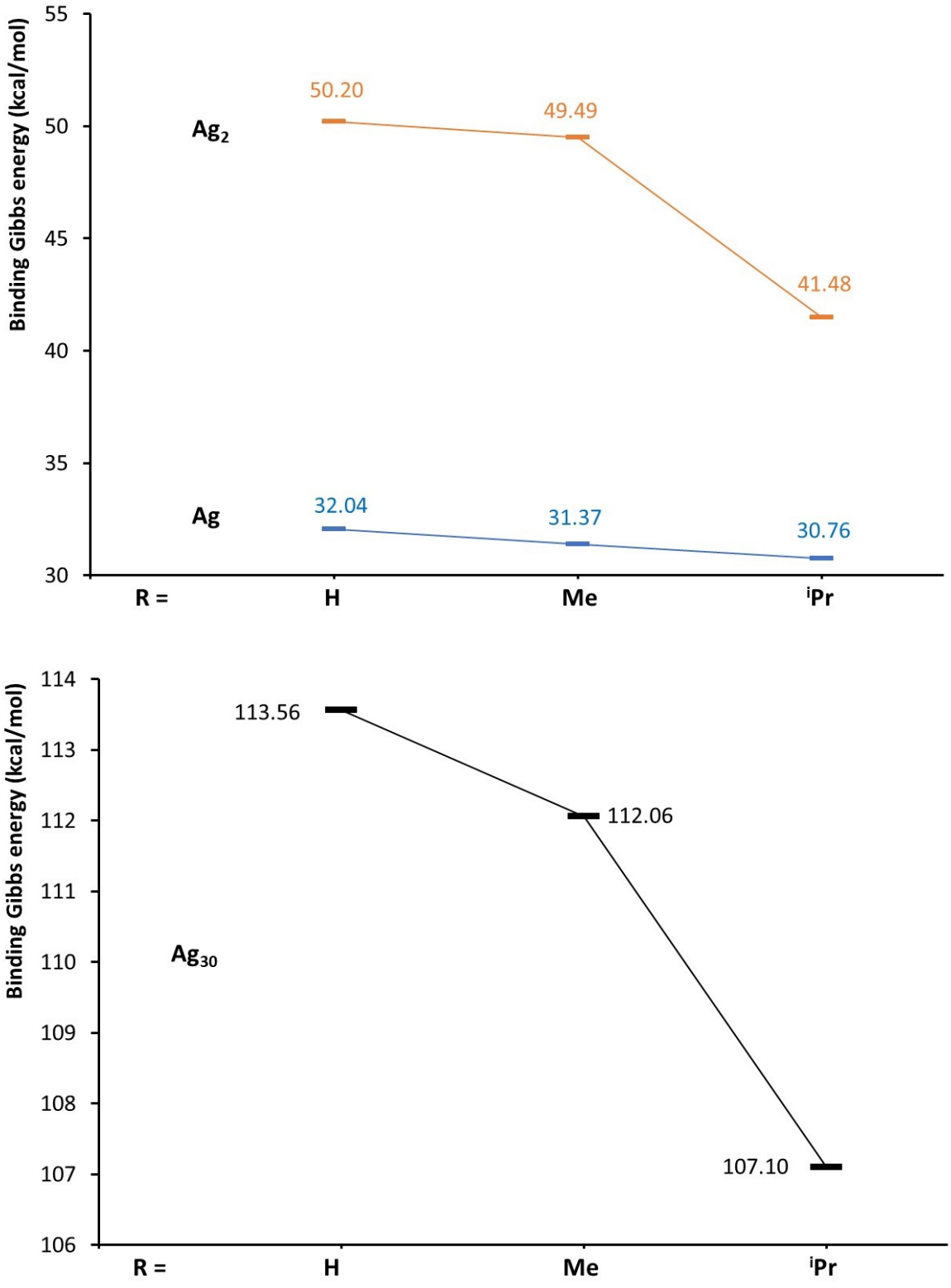


Table S1. BDE energies (kcal/mol) of the Ag-C bond in selected NHC-silver complexes and in calculated compounds $[Ag_n(NHC^R)]^{2-}$ (n = 1, 2).

Complex	BDE	References
$[Ag(NHC^H)]^{2-}$	32.0	This work
$[Ag(NHC^{Me})]^{2-}$	31.4	This work
$[Ag(NHC^{iPr})]^{2-}$	30.8	This work
[Ag(*I*Pr)(OAc)]	68.0	[1]
[Ag(S*I*Pr)(OAc)]	67.9	[1]
[Ag(*I*Ad)(OAc)]	68.4	[1]
$[Ag_2(NHC^H)]^{2-}$	50.2	This work
$[Ag_2(NHC^{Me})]^{2-}$	49.5	This work
$[Ag_2(NHC^{iPr})]^{2-}$	41.5	This work

[1] Wong, V. H. L.; Vummaleti, S. V. C.; Cavallo, L.; White, A. J. P.; Nolan, S. P.; Hii, K. K. Chem. Eur. J. 2016, 22, 13320 – 13327.

Table S2. Selected structural and energetic data of $[Ag(NHC^{R})]^{n-}$ and their corresponding $[Ag(\kappa^1\textit{O}\text{-}NHC^{R})]^{n-}$ isomers (n = 1, 2. R = H, Me, and ^{i}Pr), and selected local and integrated topological properties of the electron density at the Ag-O bond for $[Ag(\kappa^1\textit{O}\text{-}NHC^{R})]^{2-}$ complexes.

Silver(0) complex	**Ag-C distance (Å)**	**Ag-O distance (Å)**	**ΔE (kcal/mol)** [a]
$[Ag(NHC^{H})]^{2-}$	2.161	-	12.8
$[Ag(NHC^{Me})]^{2-}$	2.161	-	12.9
$[Ag(NHC^{iPr})]^{2-}$	2.164	-	13.1
$[Ag(\kappa^1\textit{O}\text{-}NHC^{H})]^{2-}$	-	2.288	
$[Ag(\kappa^1\textit{O}\text{-}NHC^{Me})]^{2-}$	-	2.293	
$[Ag(\kappa^1\textit{O}\text{-}NHC^{iPr})]^{2-}$	-	2.312	
Silver(I) complex	**Ag-C distance (Å)**	**Ag-O distance (Å)**	**ΔE (kcal/mol)** [a]
$[Ag(NHC^{H})]^{-}$	2.051	-	17.0
$[Ag(NHC^{Me})]^{-}$	2.048	-	18.8
$[Ag(NHC^{iPr})]^{-}$	2.099	-	31.9
$[Ag(\kappa^1\textit{O}\text{-}NHC^{H})]^{-}$	-	2.360	
$[Ag(\kappa^1\textit{O}\text{-}NHC^{Me})]^{-}$	-	2.354	
$[Ag(\kappa^1\textit{O}\text{-}NHC^{iPr})]^{-}$	-	2.340	

[a] Difference between the electronic energies of the $\kappa^1\textit{O}$- and the $\kappa^1\textit{C}$-isomers.

Complex	**Dist$_{(Ag\text{-}X)}$**	**ρ**	**$\nabla^2\rho$**	**δ(Ag,X)**	**$\int_{Ag\cap X}\rho$**	**|V|/G**	**H/ρ**	**Eint**
$[Ag(NHC^{H})]^{2-}$	2.288	0.056	0.232	0.533	0.497	1.091	-0.104	-21.907
$[Ag(NHC^{Me})]^{2-}$	2.293	0.055	0.229	0.528	0.496	1.092	-0.104	-21.446
$[Ag(NHC^{iPr})]^{2-}$	2.312	0.053	0.217	0.511	0.496	1.093	-0.105	-20.362

[a] All dimensions are expressed in atomic units (a.u.) except distances which are in Å and Eint, which is in kcal/mol. δ(Ag,X) means the delocalization index between Ag-X bonded atoms. $\int Ag\cap X\rho$ accounts for the integrated electron density on the whole Ag-X interatomic surface. |V|/G is an adimensional ratio at the BCP and H/ρ is the total energy ratio at the BCP.

Table S3. Selected local and integrated topological properties of the electron density at the Ag-X (X being Ag and C) for Ag_n clusters and $[Ag_n(NHC^H)]^{2-}$ complexes (n = 3 or 4).[a]

AgNP	X	$Dist_{(Ag-X)}$	ρ	$\nabla^2\rho$	δ(Ag,X)	$\int_{Ag\cap X}\rho$	|V|/G	H/ ρ	Eint
Ag_3	Ag	2.641	0.045	0.116	0.856	0.513	1.248	-0.211	-14.989
Linear	Ag	2.642	0.045	0.116	0.856	0.514	1.257	-0.211	-15.012
$[Ag_3(NHC^H)]^{2-}$ Linear	Ag	2.726	0.040	0.081	0.654	0.476	1.299	-0.218	-11.876
	Ag	2.684	0.042	0.103	0.934	0.509	1.246	-0.201	-13.444
	C	2.103	0.103	0.270	0.826	0.881	1.317	-0.305	-40.885
Ag_3	Ag	2.643(x2)	0.046	0.117	0.842	0.525	1.249	-0.209	-15.104
Triangular	Ag	3.020	0.026	0.048	0.556	0.206	1.197	-0.113	-5.581
$[Ag_3(NHC^H)]^{2-}$ Triangular	Ag	2.755	0.038	0.083	0.570	0.393	1.262	-0.193	-11.046
	Ag	2.738	0.039	0.085	0.587	0.406	1.269	-0.199	-11.438
	Ag	2.745	0.040	0.088	0.853	0.439	1.259	-0.193	-11.784
	C	2.099	0.104	0.274	0.814	0.888	1.320	-0.309	-41.554
Ag_4	Ag	2.755	0.038	0.086	0.531	0.377	1.251	-0.190	-11.253
		2.608	0.050	0.127	0.953	0.526	1.253	-0.217	-16.857
		2.787	0.036	0.077	0.488	0.346	1.254	-0.182	-10.169
		2.595	0.051	0.127	1.035	0.595	1.265	-0.224	-17.087
$[Ag_4(NHC^H)]^{2-}$	Ag	2.849	0.033	0.064	0.401	0.301	1.262	-0.174	-8.671
	Ag	2.689	0.043	0.095	0.655	0.462	1.276	-0.211	-13.098
	Ag	2.688	0.044	0.100	0.687	0.476	1.267	-0.209	-13.698
	Ag	2.639	0.047	0.113	0.943	0.556	1.264	-0.215	-15.220
	C	2.098	0.105	0.272	0.812	0.889	1.324	-0.311	-41.831

[a] All dimensions are expressed in atomic units (a.u.) except distances which are in Å and Eint are in kcal/mol. δ(Ag,X) means the delocalization index between Ag-X bonded atoms. $\int_{Ag\cap X}\rho$ accounts for the integrated electron density over the whole Ag-X interatomic surface. |V|/G is an adimensional ratio at the BCP and H_{BCP}/ρ_{BCP} is the total energy ratios at the BCP.

Table S4. Selected structural data and relative energy data of $[Ag_{20}(NHC^{R})]^{2-}$ (R = H, Me, and ^{i}Pr) for the three different coordination types.

$[Ag_{20}(NHC^{H})]^{2-}$	Face	Vertex	Edge
Relative ΔG (kcal/mol)	3.75	0.00	10.39
Ag-C (Å)	2.212	2.145	2.172
Ag-O (Å)	2.250	2.482, 2.533	2.222, 2.313
$[Ag_{20}(NHC^{Me})]^{2-}$	**Face**	**Vertex**	**Edge**
Relative ΔG (kcal/mol)	1.44	2.10	0.00
Ag-C (Å)	2.206	2.231	2.198
Ag-O (Å)	2.254	2.322, 2.417	2.219, 2.307
$[Ag_{20}(NHC^{Me})]^{2-}$	**Face**	**Vertex**	**Edge**
Relative ΔG (kcal/mol)	3.73	9.72	0.00
Ag-C (Å)	2.205	2.140	2.220
Ag-O (Å)	2.261	2.486, 2.554	2.223, 2.315

Table S5. Selected local and integrated topological properties of the electron density at the Ag-X (X being Ag and C) for $[Ag_{20}(NHC^{R})]^{2-}$ complexes (R = Me, ^{i}Pr).[a]

AgNP	X	$Dist_{(Ag-X)}$	ρ_{BCP}	$\nabla^2\rho_{BCP}$	δ(Ag,X)	|V|/G	H/ρ	Eint
$[Ag_{20}(NHC^{Me})]^{2-}$ F	C	2.207	0.083	0.233	0.647	1.253	-0.237	-30.734
	O	2.254	0.059	0.261	0.447	1.081	-0.098	-24.148
	O	2.254	0.059	0.261	0.447	1.081	-0.098	-24.148
	H	2.473	0.018	0.043	0.077	0.987	0.007	-3.136
	H	2.473	0.018	0.043	0.077	0.987	0.007	-3.136
$[Ag_{20}(NHC^{Me})]^{2-}$ V	C	2.231	0.078	0.229	0.570	1.234	-0.224	-28.853
	O	2.322	0.052	0.215	0.382	1.088	-0.099	-20.071
	O	2.417	0.042	0.165	0.304	1.080	-0.086	-15.054
	O	2.554	0.031	0.116	0.250	1.053	-0.052	-10.663
	H	2.640	0.013	0.033	0.054	0.933	0.041	-2.195
	H	2.545	0.015	0.043	0.066	0.952	0.032	-3.136
$[Ag_{20}(NHC^{Me})]^{2-}$ E	C	2.198	0.084	0.244	0.615	1.247	-0.238	-31.675
	O	2.219	0.063	0.289	0.462	1.081	-0.101	-26.657
	O	2.307	0.053	0.224	0.392	1.081	-0.093	-20.699
	H	2.637	0.014	0.039	0.055	0.938	0.042	-2.823
	H	2.665	0.014	0.038	0.047	0.922	0.050	-2.509
	H	2.666	0.013	0.037	0.042	0.924	0.050	-2.509
	H	2.751	0.012	0.024	0.046	0.943	0.028	-1.568
$[Ag_{20}(NHC^{iPr})]^{2-}$ F	C	2.205	0.084	0.233	0.644	1.254	-0.237	-30.734
	O	2.261	0.058	0.255	0.438	1.083	-0.099	-23.521
	O	2.261	0.058	0.255	0.438	1.083	-0.099	-23.521
	H	2.478	0.018	0.043	0.073	0.992	0.004	-3.136
	H	2.478	0.018	0.043	0.073	0.992	0.004	-3.136
	H	2.734	0.010	0.020	0.060	0.934	0.037	-1.568
	H	2.734	0.010	0.020	0.060	0.934	0.037	-1.568
$[Ag_{20}(NHC^{iPr})]^{2-}$ V	C	2.140	0.096	0.268	0.710	1.284	-0.278	-37.634
	O	2.486	0.037	0.139	0.274	1.083	-0.085	-12.858
	O	2.554	0.033	0.119	0.236	1.071	-0.070	-10.663
	C	2.980	0.015	0.047	0.036	0.945	0.040	-3.136
	H	2.825	0.010	0.025	0.048	0.891	0.062	-1.568
$[Ag_{20}(NHC^{iPr})]^{2-}$ E	C	2.188	0.086	0.253	0.632	1.249	-0.243	-32.930
	O	2.198	0.066	0.308	0.474	1.082	-0.104	-28.539
	O	2.285	0.054	0.241	0.388	1.067	-0.081	-21.640
	H	2.405	0.021	0.054	0.082	1.024	-0.016	-4.391
	H	2.484	0.016	0.040	0.064	0.972	0.017	-2.823
	H	3.514	0.003	0.009	0.016	0.725	0.147	-0.314
	H	2.557	0.018	0.047	0.069	0.996	0.002	-2.823

[a] For units and definitions see the footnote of Table S3.

Table S6. Selected local and integrated topological properties of the electron density at the Ag-X (X being Ag and C) for $[Ag_{30}(NHC^{R})]^{2-}$ complexes (R = H, Me, ^{i}Pr).[a]

AgNP	X	$Dist_{(Ag-X)}$	ρ_{BCP}	$\nabla^2\rho_{BCP}$	δ(Ag,X)	|V|/G	H/ρ	Eint
$[Ag_{30}(NHC^{H})]^{2-}$	C	2.119	0.099	0.284	0.713	1.288	-0.288	-40.143
	O	2.232	0.061	0.278	0.454	1.080	-0.098	-25.403
	O	2.327	0.048	0.206	0.350	1.069	-0.080	-18.503
	O	2.357	0.045	0.190	0.349	1.066	-0.074	-16.935
$[Ag_{30}(NHC^{Me})]^{2-}$	C	2.120	0.099	0.282	0.708	1.288	-0.288	-39.829
	O	2.233	0.061	0.276	0.453	1.081	-0.099	-25.403
	O	2.335	0.047	0.202	0.345	1.070	-0.079	-18.190
	O	2.348	0.046	0.195	0.354	1.067	-0.075	-17.562
	H	2.704	0.012	0.033	0.117	0.916	0.053	-2.195
	H	2.841	0.010	0.020	0.077	0.937	0.029	-1.254
$[Ag_{30}(NHC^{iPr})]^{2-}$	C	2.124	0.098	0.279	0.703	1.287	-0.286	-39.516
	O	2.234	0.061	0.274	0.450	1.084	-0.102	-25.403
	O	2.360	0.045	0.187	0.333	1.071	-0.080	-16.935
	O	2.333	0.047	0.203	0.358	1.066	-0.075	-18.190
	H	2.665	0.013	0.035	0.042	0.930	0.045	-2.509
	H	3.088	0.006	0.013	0.035	0.873	0.063	-0.627
	H	2.729	0.012	0.025	0.051	0.955	0.022	-1.882

[a] For units and definitions see the footnote of Table S3.

Table S7. Coordinates of the optimized compounds.

$[Ag(NHC^{H})]^{2-}$

Ag	0.000018	2.207939	-0.103128
O	3.335403	-2.428726	-0.566432
O	-4.746977	-0.685235	-0.174281
O	-3.335474	-2.428636	-0.566482
N	1.081351	-0.765302	0.237077
N	-1.081384	-0.765278	0.237070
C	-0.000007	0.056853	0.105298
C	-0.683612	-2.073417	0.462057
H	-1.427791	-2.860497	0.495323
C	0.683547	-2.073434	0.462052
H	1.427708	-2.860532	0.495316
C	2.473466	-0.291731	0.262442
H	2.506506	0.628819	-0.334910
C	3.625136	-1.253440	-0.222938
C	-2.473488	-0.291672	0.262427
H	-2.723757	-0.005921	1.296620
C	-3.625181	-1.253351	-0.222966
O	4.746944	-0.685345	-0.174272
H	-2.506502	0.628880	-0.334923
H	2.723736	-0.005982	1.296636

$[Ag(NHC^{Me})]^{2-}$

Ag	-0.000011	2.219021	-0.000081
O	3.378995	-2.296438	-0.825440
O	-4.699717	-0.475612	0.487833
O	-3.379109	-2.296867	0.824616
N	1.080411	-0.773547	0.054008
N	-1.080381	-0.773542	-0.054023
C	0.000016	0.057768	0.000063
C	-0.681896	-2.101835	-0.040711
H	-1.429785	-2.885307	-0.022233
C	0.681932	-2.101838	0.040460
H	1.429794	-2.885326	0.021807
C	2.461382	-0.290928	0.248555
H	2.477123	0.716525	-0.191928
C	3.619396	-1.120353	-0.444995
C	-2.461371	-0.290884	-0.248358
H	-2.477072	0.716508	0.192254
C	-3.619330	-1.120433	0.445118
O	4.699964	-0.475774	-0.486878
C	2.754241	-0.173100	1.747823
H	2.697917	-1.162863	2.227848
H	3.770039	0.224116	1.874051
H	2.028539	0.497202	2.235205
C	-2.754399	-0.172887	-1.747582
H	-2.028704	0.497410	-2.234983
H	-2.698223	-1.162610	-2.227703
H	-3.770174	0.224443	-1.873666

$[Ag(NHC^{iPr})]^{2-}$

Ag	0.053650	2.182403	-0.122338
O	3.369552	-2.510137	-0.987765
O	-4.257212	-0.408970	1.836399
O	-3.377923	-2.369301	1.096043
N	1.099101	-0.830830	-0.050580
N	-1.042019	-0.784589	0.246167
C	0.037085	0.022892	0.022367
C	-0.661164	-2.117263	0.307303
H	-1.417787	-2.872327	0.493897
C	0.693333	-2.145120	0.130486
H	1.423127	-2.943945	0.055528
C	2.497263	-0.401250	-0.196961
H	2.446993	0.634723	-0.563122
C	3.308527	-1.273405	-1.243027
C	-2.420146	-0.256480	0.333842

H	-2.321177	0.720943	0.826326
C	-3.436029	-1.110824	1.191998
O	3.854866	-0.625299	-2.169361
C	3.226624	-0.434882	1.165510
H	3.314506	-1.503109	1.432337
C	-2.964946	0.000436	-1.095526
H	-2.187365	0.608294	-1.595737
C	4.638793	0.136390	1.007145
H	5.198253	0.057728	1.954278
H	5.194680	-0.389613	0.219036
H	4.591764	1.201745	0.727315
C	2.464199	0.301723	2.268681
H	2.297695	1.357072	1.995877
H	1.476239	-0.143000	2.450450
H	3.032467	0.274866	3.214231
C	-4.250385	0.829124	-1.046807
H	-4.076005	1.787808	-0.535867
H	-4.607730	1.039635	-2.068963
H	-5.037077	0.300243	-0.489471
C	-3.157885	-1.287398	-1.899967
H	-2.215643	-1.847729	-1.985598
H	-3.889848	-1.945565	-1.408885
H	-3.508710	-1.051541	-2.918670

$[Ag(NHC^{H})]^{-}$ silver(I)

Ag	0.000283	2.097181	-0.059334
O	3.270819	-2.348759	-0.541013
O	-4.585229	-0.485378	-0.635359
O	-3.271450	-2.348124	-0.541085
N	1.090555	-0.717601	0.410876
N	-1.090645	-0.717380	0.410685
C	0.000046	0.078299	0.301429
C	-0.686368	-2.024519	0.599535
H	-1.435937	-2.808500	0.618848
C	0.685975	-2.024663	0.599594
H	1.435349	-2.808826	0.618959
C	2.481298	-0.245942	0.380249
H	2.473435	0.751233	-0.081669
C	3.551705	-1.137890	-0.366977
C	-2.481283	-0.245378	0.379890
H	-2.832961	-0.136861	1.417971
C	-3.551966	-1.137151	-0.367158
O	4.585098	-0.486344	-0.635231
H	-2.473131	0.751683	-0.082267
H	2.832980	-0.137786	1.418366

$[Ag(NHC^{Me})]^{-}$ silver(I)

Ag	-0.000026	2.084957	-0.000359
O	-4.380470	-0.164829	0.948394
O	3.463797	-2.222842	-0.583356
O	4.380893	-0.164902	-0.947830
N	-1.076777	-0.766065	-0.171549
N	1.076847	-0.765991	0.171408
C	0.000032	0.036897	-0.000217
C	0.676975	-2.087772	0.108731
H	1.427023	-2.869406	0.162033
C	-0.676815	-2.087820	-0.108877
H	-1.426827	-2.869493	-0.162159
C	-2.444777	-0.288487	-0.430747
H	-2.428451	0.785592	-0.186408
C	-3.540260	-0.970987	0.488473
C	2.444796	-0.288325	0.430706
H	2.428480	0.785711	0.186176
C	3.540419	-0.970966	-0.488230
O	-3.463697	-2.222863	0.583667
C	2.806882	-0.492047	1.900037
H	2.075274	-0.012602	2.570107
C	-2.807028	-0.492476	-1.899998
H	-2.851276	-1.566207	-2.129501
H	-3.800597	-0.061314	-2.084954
H	-2.075498	-0.013156	-2.570244
H	3.800432	-0.060855	2.085026

H	2.851097	-1.565734	2.129762

[Ag(NHC^{iPr})]$^{-}$ silver(I)

Ag	0.510618	-1.828249	-0.573947
O	-3.597683	2.459573	0.129673
O	2.395940	-1.820934	0.694153
O	3.208333	-0.214576	2.058509
N	-1.216240	0.829357	-0.084357
N	0.946112	0.923158	0.039146
C	-0.088175	0.179912	-0.460958
C	0.455859	2.014316	0.738323
H	1.102041	2.732810	1.225961
C	-0.908369	1.961625	0.653184
H	-1.720220	2.613012	0.965969
C	-2.566952	0.316485	-0.397127
H	-2.454689	-0.206157	-1.356051
C	-3.677012	1.429221	-0.592268
C	2.351302	0.493523	-0.094444
H	2.404601	-0.003188	-1.077211
C	2.686555	-0.601454	1.004554
O	-4.549736	1.098310	-1.428119
C	-2.980471	-0.728551	0.668409
H	-2.122417	-1.429220	0.743408
C	3.332291	1.669931	-0.099501
H	3.287582	2.143981	0.895414
C	2.994422	2.692988	-1.190008
H	1.979664	3.100337	-1.089475
H	3.703701	3.534230	-1.160683
H	3.069360	2.229558	-2.187149
C	4.759469	1.146570	-0.293751
H	5.042224	0.467637	0.519833
H	4.848013	0.607484	-1.251561
H	5.473459	1.983683	-0.316061
C	-3.210052	-0.114597	2.051059
H	-4.021580	0.626201	2.014914
H	-3.473998	-0.899567	2.776878
H	-2.310044	0.397544	2.420542
C	-4.200345	-1.524917	0.201334
H	-4.005358	-2.020859	-0.761397
H	-4.459033	-2.295665	0.944657
H	-5.062657	-0.861009	0.051477

[Ag(NHC^{H})]$^{2-}$ κ^1-O coordination

Ag	4.376985	-0.197996	-0.127563
O	1.314392	-0.897471	-0.007843
O	-6.853891	0.097596	-0.729293
O	-5.369772	-1.584280	-0.337225
N	-1.157003	0.602251	0.343274
N	-3.279381	0.411620	0.146540
C	-2.251879	1.269890	-0.157186
C	-2.848924	-0.724161	0.820543
H	-3.542966	-1.527518	1.040323
C	-1.495073	-0.602933	0.949694
H	-0.740304	-1.285229	1.321530
C	0.159789	1.220624	0.378453
H	0.134438	2.042255	-0.347663
C	1.407711	0.336675	0.104998
C	-4.685076	0.753037	-0.098758
H	-5.081533	1.273508	0.790590
C	-5.725392	-0.380679	-0.430105
O	2.473411	1.057620	0.063486
H	-4.686274	1.483554	-0.916518
H	0.327710	1.679468	1.369012

[Ag(NHC^{Me})]$^{2-}$ κ^1-O coordination

Ag	4.561580	-0.393989	0.141795
O	1.605168	-0.119362	1.121229
O	-6.648721	0.095832	-0.621966

O	-5.482863	0.442990	1.301493
N	-0.941864	0.419933	-0.202251
N	-3.025522	-0.067752	-0.183389
C	-1.995302	0.181088	-1.054848
C	-2.632445	0.007880	1.147780
H	-3.357313	-0.113021	1.944294
C	-1.307118	0.332345	1.138315
H	-0.582529	0.453347	1.934036
C	0.345698	0.891369	-0.710045
H	0.337472	0.628190	-1.774939
C	1.617571	0.258033	-0.065312
C	-4.352403	-0.496239	-0.651378
H	-4.399040	-0.162489	-1.695550
C	-5.611195	0.099549	0.095911
O	2.616209	0.269827	-0.875379
C	0.449931	2.418088	-0.575979
H	0.439403	2.709432	0.485054
H	1.389918	2.766377	-1.026997
H	-0.404192	2.895111	-1.079661
C	-4.447170	-2.026822	-0.615862
H	-3.629408	-2.481529	-1.197817
H	-4.380319	-2.388416	0.422280
H	-5.416847	-2.335179	-1.031946

$[Ag(NHC^{iPr})]^{2-}$ κ^1-O coordination

Ag	4.786051	-0.972348	-0.097519
O	2.234328	0.146284	1.230902
O	-6.114974	0.670942	-0.111071
O	-4.933113	0.055943	1.729896
N	-0.438982	0.673085	-0.007405
N	-2.529576	0.217469	0.021050
C	-1.521687	0.556885	-0.848822
C	-2.094644	0.123538	1.338724
H	-2.801677	-0.109458	2.127723
C	-0.763800	0.424994	1.323727
H	-0.010232	0.440926	2.102382
C	0.854441	1.169763	-0.472229
H	0.797457	1.129873	-1.568048
C	2.066009	0.307425	0.003617
C	-3.886814	-0.081155	-0.471856
H	-3.999307	0.543267	-1.367223
C	-5.084208	0.268968	0.494379
O	2.827101	-0.087901	-0.948637
C	1.085640	2.634240	-0.020897
H	1.133332	2.608835	1.081928
C	-3.957021	-1.561468	-0.935142
H	-3.075135	-1.695474	-1.588751
C	-0.064768	3.546411	-0.449374
H	-0.146163	3.579958	-1.547803
H	-1.029286	3.189047	-0.065692
H	0.102006	4.574053	-0.084848
C	2.424910	3.159322	-0.544984
H	3.265918	2.540985	-0.202177
H	2.438207	3.153769	-1.647325
H	2.591577	4.195915	-0.208468
C	-3.846244	-2.555629	0.224212
H	-3.865468	-3.591816	-0.154724
H	-2.908197	-2.412288	0.779301
H	-4.674655	-2.416285	0.934701
C	-5.217166	-1.820395	-1.765070
H	-6.121487	-1.620794	-1.171958
H	-5.255242	-1.154531	-2.640888
H	-5.237324	-2.865355	-2.119924

$[Ag_2(NHC^{H})]^{2-}$

Ag	0.950600	-0.000673	-0.004330
Ag	3.599084	-0.001783	-0.108402
O	-1.895981	4.747576	-0.171863
O	-3.629555	-3.328153	-0.601640
O	-3.626561	3.330822	-0.603163
N	-1.977681	-1.081815	0.239037

N	-1.976686	1.083390	0.238502
C	-1.153092	0.000384	0.138169
C	-3.290967	0.685181	0.414091
H	-4.076738	1.431591	0.418691
C	-3.291592	-0.682315	0.414450
H	-4.078057	-1.427988	0.419430
C	-1.508227	-2.475778	0.275740
H	-0.576946	-2.514777	-0.304390
C	-2.464482	-3.624694	-0.231570
C	-1.505957	2.476947	0.274499
H	-1.244141	2.727310	1.314573
C	-2.461167	3.626473	-0.233382
O	-1.900363	-4.746297	-0.169363
H	-0.574640	2.514793	-0.305646
H	-1.246633	-2.725854	1.315939

$[Ag_2(NHC^{Me})]^{2-}$

Ag	1.013583	-0.002540	-0.000175
Ag	3.662558	-0.006560	-0.000494
O	-1.638503	-4.690360	-0.520907
O	-3.458647	3.377862	0.808568
O	-3.469135	-3.369749	-0.807758
N	-1.922373	1.083493	-0.054986
N	-1.925643	-1.079678	0.054804
C	-1.094718	0.000660	-0.000017
C	-3.251734	-0.678125	0.040711
H	-4.034635	-1.426745	0.022763
C	-3.249660	0.685937	-0.041133
H	-4.030371	1.436831	-0.023161
C	-1.440678	2.465795	-0.244536
H	-0.434461	2.483788	0.198262
C	-2.274904	3.619028	0.454134
C	-1.448031	-2.463429	0.244361
H	-0.442092	-2.484536	-0.198932
C	-2.285968	-3.614303	-0.453704
O	-1.624262	4.693168	0.521258
C	-1.326000	2.766502	-1.742090
H	-2.317709	2.718766	-2.218471
H	-0.924096	3.780865	-1.863509
H	-0.661759	2.041672	-2.238879
C	-1.333491	-2.764164	1.741924
H	-0.666816	-2.041218	2.238194
H	-2.324814	-2.713314	2.218786
H	-0.934583	-3.779704	1.863374

$[Ag_2(NHC^{iPr})]^{2-}$

Ag	0.930191	-0.450267	-0.258337
Ag	2.848903	-2.212140	0.300386
O	1.265424	4.073163	-1.913503
O	-4.633139	-0.529213	-1.556032
O	1.684127	1.847149	-1.667309
N	-2.194414	0.295879	-0.278061
N	-0.917007	2.036906	-0.181970
C	-0.878888	0.674106	-0.207698
C	-2.224390	2.496340	-0.240023
H	-2.454888	3.555431	-0.258477
C	-3.032777	1.398520	-0.301723
H	-4.095385	1.259704	-0.460138
C	-2.646639	-1.105050	-0.235441
H	-1.792343	-1.690054	-0.602893
C	-3.898496	-1.465663	-1.140483
C	0.237735	2.940302	-0.071516
H	-0.191126	3.950867	0.014877
C	1.148454	2.946188	-1.366328
O	-4.036181	-2.706328	-1.286809
C	-2.946920	-1.573702	1.213773
H	-3.206842	-2.635433	1.072200
C	1.066254	2.641746	1.190643
H	1.472710	1.620508	1.063621
C	-4.161700	-0.865466	1.822402
H	-5.035790	-0.936381	1.159307

H	-4.418660	-1.312626	2.797230
H	-3.949675	0.202775	1.991362
C	-1.736678	-1.478895	2.143680
H	-0.854767	-1.983901	1.722437
H	-1.444843	-0.431357	2.317708
H	-1.968613	-1.930931	3.123595
C	0.211442	2.672064	2.458751
H	-0.619887	1.955560	2.398673
H	0.815589	2.414079	3.343475
H	-0.215052	3.677650	2.620728
C	2.244473	3.610939	1.292397
H	2.883677	3.545313	0.402000
H	1.891074	4.653069	1.375287
H	2.853412	3.382754	2.181960

$[Ag_3(NHC^H)]^{2-}$ linear

Ag	0.369873	-0.000813	-0.023216
Ag	-2.354343	-0.000963	-0.112357
Ag	-5.034395	-0.000608	0.040779
O	3.199441	-4.737358	-0.218444
O	4.951687	3.322227	-0.566050
O	4.953430	-3.323060	-0.556238
N	3.283668	1.084356	0.254295
N	3.284183	-1.083757	0.257415
C	2.466321	-0.000052	0.146782
C	4.595563	-0.683165	0.445374
H	5.380328	-1.430868	0.459493
C	4.595228	0.684934	0.443488
H	5.379628	1.433056	0.455530
C	2.813125	2.478702	0.273608
H	1.885487	2.512091	-0.312597
C	3.773727	3.621200	-0.243135
C	2.814335	-2.478271	0.280732
H	2.550389	-2.736906	1.318138
C	3.775564	-3.621728	-0.232696
O	3.197048	4.736577	-0.231934
H	1.886733	-2.513820	-0.305403
H	2.549067	2.740174	1.310274

$[Ag_3(NHC^H)]^{2-}$ triangular

Ag	-0.310604	-0.000144	0.028891
Ag	-2.702534	0.001176	-1.337700
Ag	-2.676984	-0.001773	1.406855
O	2.519639	4.746148	0.194666
O	4.280418	-3.340846	0.527909
O	4.279510	3.340660	0.535182
N	2.602635	-1.083335	-0.234398
N	2.602440	1.084099	-0.232201
C	1.782572	0.000197	-0.124038
C	3.913664	0.684799	-0.422894
H	4.697794	1.433104	-0.439017
C	3.913752	-0.683424	-0.424507
H	4.697991	-1.431579	-0.442348
C	2.128070	-2.476548	-0.258105
H	1.218659	-2.515389	0.355980
C	3.097309	-3.630432	0.214023
C	2.127578	2.477268	-0.253101
H	1.829421	2.725130	-1.283723
C	3.096370	3.630481	0.221627
O	2.520904	-4.746214	0.184934
H	1.218039	2.514588	0.360885
H	1.829801	-2.722337	-1.289191

$[Ag_4(NHC^H)]^{2-}$

Ag	0.757506	-0.146092	1.162962
Ag	-2.091043	-0.139936	1.142525
Ag	-0.684303	-0.417005	3.416514
Ag	-4.153970	0.041622	-0.493022

O	3.229760	4.730275	0.309566
O	4.812215	-3.288571	-0.908908
O	4.066799	3.593006	-1.479480
N	3.059110	-1.013905	-0.754100
N	3.230289	1.093260	-0.274170
C	2.459474	-0.009462	-0.055448
C	4.297867	0.782955	-1.096770
H	4.969645	1.568919	-1.420101
C	4.188433	-0.546412	-1.400481
H	4.826057	-1.234004	-1.941208
C	2.545448	-2.383992	-0.860886
H	1.837971	-2.526699	-0.033558
C	3.588931	-3.571655	-0.849584
C	3.022219	2.394484	0.379155
H	1.947412	2.482126	0.586785
C	3.493511	3.705282	-0.366124
O	3.014104	-4.687435	-0.813540
H	3.541051	2.381961	1.350128
H	1.974466	-2.473159	-1.798533

$[Ag_{20}(NHC^{H})]^{2-}$ face

Ag	-0.473146	0.000953	-1.843490
Ag	-2.817848	1.520070	-1.836197
Ag	1.940179	1.333671	-1.688178
Ag	-0.375390	-2.924402	-1.698904
Ag	-0.375350	2.926040	-1.695988
Ag	-2.817810	-1.518275	-1.837678
Ag	1.940100	-1.332095	-1.689487
Ag	2.225401	4.025647	-1.374583
Ag	2.225347	-4.024391	-1.378698
Ag	-5.170125	0.000922	-1.928593
Ag	1.073180	2.739479	0.716744
Ag	-1.356687	1.458037	0.544873
Ag	0.251003	1.379180	2.863841
Ag	-3.773308	-0.000295	0.432734
Ag	-2.305630	-0.001449	2.761324
Ag	-0.773445	-0.002611	5.047939
Ag	2.060327	-0.000607	0.953066
Ag	0.251039	-1.382312	2.862542
Ag	1.073173	-2.740471	0.714042
Ag	-1.356390	-1.458310	0.543338
O	4.412064	-4.341580	-0.953518
O	6.428068	3.351169	-0.796616
O	6.427975	-3.350319	-0.800421
N	5.079090	1.078827	0.481135
N	5.079100	-1.079461	0.479988
C	4.248142	-0.000400	0.629681
C	6.390274	-0.681563	0.269413
H	7.158359	-1.419416	0.074361
C	6.390269	0.681166	0.270141
H	7.158348	1.419238	0.075894
C	4.649250	2.474539	0.573000
H	3.551426	2.466153	0.551278
C	5.222658	3.445980	-0.509670
C	4.649276	-2.475271	0.570367
H	4.958040	-2.883347	1.547810
C	5.222618	-3.445535	-0.513392
O	4.412099	4.342413	-0.948995
H	3.551451	-2.466871	0.548728
H	4.957946	2.881554	1.550906

$[Ag_{20}(NHC^{H})]^{2-}$ vertex

Ag	2.483369	-0.049750	-0.121393
Ag	2.488408	-2.295838	1.579795
Ag	2.109837	-0.390951	-2.890563
Ag	2.455562	2.537988	0.982216
Ag	2.295136	-2.677457	-1.120805
Ag	2.515677	0.391287	2.659560
Ag	2.244939	2.134747	-1.877566
Ag	2.090831	-2.975043	-3.833147
Ag	2.345592	4.658341	-0.773510

Ag	2.676397	-1.830832	4.270140
Ag	-0.211937	-2.022391	-2.497534
Ag	0.021860	-1.746002	0.295797
Ag	-2.372163	-1.021828	-1.038524
Ag	0.188532	-1.237657	3.060998
Ag	-2.182244	-0.636318	1.699890
Ag	-4.588105	-0.140262	0.391152
Ag	-0.163797	0.632687	-1.499928
Ag	-2.329122	1.747890	-0.016882
Ag	0.002366	3.205824	-0.401197
Ag	0.051804	1.032590	1.374898
O	-4.137276	2.928629	1.206416
O	-10.011420	-1.928761	0.335387
O	-4.489827	2.624701	-1.006820
N	-7.693210	-0.348999	-0.233392
N	-7.110939	1.711090	0.021198
C	-6.637035	0.434459	0.121839
C	-8.433209	1.715743	-0.394344
H	-8.992130	2.635579	-0.522850
C	-8.801534	0.411571	-0.556208
H	-9.742483	-0.078470	-0.778090
C	-7.660090	-1.815857	-0.311724
H	-7.444529	-2.105573	-1.351545
C	-8.966389	-2.597541	0.120253
C	-6.395740	2.922304	0.423036
H	-6.799118	3.754414	-0.172934
C	-4.872180	2.825098	0.179586
O	-8.771266	-3.833260	0.154168
H	-6.578761	3.117015	1.489084
H	-6.817681	-2.150901	0.305413

$[Ag_{20}(NHC^{H})]^{2-}$ edge

Ag	-2.311290	-0.793777	-0.694970
Ag	-3.645172	-0.073840	1.689870
Ag	-2.091394	1.047983	-2.801506
Ag	-0.783396	-3.170566	-0.807403
Ag	-3.616852	1.693002	-0.399997
Ag	-2.149397	-2.567160	1.482877
Ag	-0.742132	-1.330152	-2.986563
Ag	-3.503134	3.427897	-2.504682
Ag	0.553571	-3.737673	-3.128175
Ag	-3.591369	-1.871468	3.747303
Ag	-1.123409	3.103104	-1.056783
Ag	-1.287613	1.386899	1.168463
Ag	1.136505	2.685162	0.479644
Ag	-1.186329	-0.514640	3.239813
Ag	1.116617	0.893483	2.608912
Ag	3.379966	2.341474	2.051161
Ag	0.322926	0.643943	-1.281187
Ag	2.736040	0.235064	0.240185
Ag	1.753160	-1.791833	-1.460264
Ag	0.280120	-1.162997	0.879009
O	3.508670	-3.160068	-2.088620
O	5.507122	2.965677	2.201386
O	5.625927	-3.913667	-1.809376
N	5.915318	0.644787	-0.095875
N	5.413660	-1.443240	-0.020785
C	4.852966	-0.201775	0.027380
C	6.787940	-1.376029	-0.177663
H	7.385861	-2.271229	-0.296725
C	7.108461	-0.049994	-0.213836
H	8.059024	0.466569	-0.267368
C	5.822881	2.099257	-0.048372
H	6.425611	2.512551	-0.869621
C	6.373896	2.656425	1.302885
C	4.652887	-2.687651	-0.005915
H	5.150150	-3.392026	0.675910
C	4.598170	-3.320911	-1.433316
O	7.609194	2.747494	1.400812
H	3.651382	-2.445624	0.373553
H	4.765908	2.355688	-0.199946

$[Ag_{20}(NHC^{Me})]^{2-}$ face

Ag	-0.465075	0.000953	-1.838405
Ag	-2.803198	1.525454	-1.783033
Ag	1.948459	1.331297	-1.720773
Ag	-0.355659	-2.930053	-1.689831
Ag	-0.355686	2.931721	-1.686792
Ag	-2.803142	-1.523712	-1.784589
Ag	1.948427	-1.329578	-1.722123
Ag	2.270405	4.013481	-1.417223
Ag	2.270452	-4.012073	-1.421457
Ag	-5.153477	0.000860	-1.836943
Ag	1.127080	2.751853	0.700815
Ag	-1.296291	1.455764	0.568640
Ag	0.346251	1.382327	2.862672
Ag	-3.716942	-0.000363	0.500291
Ag	-2.209197	-0.001541	2.802812
Ag	-0.635430	-0.002714	5.063178
Ag	2.091912	-0.000577	0.926521
Ag	0.346295	-1.385529	2.861295
Ag	1.127114	-2.752793	0.697980
Ag	-1.296061	-1.456222	0.567072
O	4.480845	-4.289173	-1.077555
O	6.524869	3.492720	-0.577608
O	6.524869	-3.491856	-0.581498
N	5.087269	1.078980	0.370383
N	5.087240	-1.079548	0.369284
C	4.266408	-0.000369	0.554814
C	6.388575	-0.681975	0.101920
H	7.152195	-1.422909	-0.102143
C	6.388631	0.681638	0.102787
H	7.152305	1.422765	-0.100366
C	4.645000	2.473474	0.535901
H	3.557958	2.443863	0.364246
C	5.284064	3.480808	-0.479673
C	4.644949	-2.474200	0.533369
C	4.908470	-2.952947	1.960191
C	5.284088	-3.480481	-0.483191
O	4.480775	4.290244	-1.072955
H	3.557913	-2.444415	0.361708
C	4.908554	2.950754	1.963210
H	4.485955	3.956683	2.097588
H	4.430740	2.270158	2.682825
H	5.990151	2.994331	2.154200
H	4.485880	-3.959020	2.093526
H	5.990062	-2.996706	2.151169
H	4.430627	-2.273094	2.680488

$[Ag_{20}(NHC^{Me})]^{2-}$ vertex

Ag	1.984886	0.511655	-0.379402
Ag	2.789328	-1.121452	1.774777
Ag	1.652243	-0.609639	-2.930673
Ag	0.992748	3.106500	0.124732
Ag	2.650727	-2.206980	-0.727341
Ag	1.941100	1.615229	2.205318
Ag	0.805804	1.961358	-2.493765
Ag	2.447700	-3.240915	-3.250417
Ag	0.121148	4.579339	-2.023120
Ag	2.869135	0.024817	4.259975
Ag	0.024419	-2.795489	-1.893950
Ag	0.246948	-1.797157	0.721179
Ag	-2.302825	-2.277454	-0.431550
Ag	0.314687	-0.553348	3.242676
Ag	-2.159502	-1.143004	2.095115
Ag	-4.684053	-1.460600	0.900459
Ag	-0.788239	-0.116085	-1.529081
Ag	-3.128422	0.471125	-0.134898
Ag	-1.632812	2.624506	-1.046275
Ag	-0.633610	1.029057	1.102429
O	-4.154474	2.600302	-0.641002
O	-6.414809	-3.007991	0.900273
O	-4.608039	4.418425	0.643643
N	-7.157419	-0.420148	-0.570935

N	-6.500542	1.378940	0.413014
C	-6.188387	0.058448	0.263745
C	-7.625898	1.714971	-0.321163
H	-8.018200	2.725192	-0.341667
C	-8.043594	0.575945	-0.941461
H	-8.887746	0.386441	-1.594228
C	-7.276046	-1.811623	-1.050047
H	-8.237001	-1.847304	-1.579838
C	-7.413822	-2.859614	0.120878
C	-5.769047	2.407236	1.170403
H	-6.533696	3.131003	1.488029
C	-4.750699	3.234557	0.302089
O	-8.492771	-3.483206	0.145196
C	-5.078662	1.852532	2.410463
H	-4.256845	1.169367	2.146939
C	-6.145528	-2.160544	-2.013356
H	-5.172465	-2.165227	-1.495895
H	-5.785280	1.297701	3.045200
H	-4.656969	2.694413	2.974934
H	-6.088854	-1.436382	-2.840341
H	-6.313100	-3.166239	-2.424453

$[Ag_{20}(NHC^{Me})]^{2-}$ edge

Ag	0.131175	-1.701628	0.484763
Ag	-1.121314	-2.612403	-1.900644
Ag	2.837401	-0.698707	0.612072
Ag	-1.548289	-1.497556	2.808329
Ag	1.528821	-1.685625	-1.911301
Ag	-2.620938	-2.478174	0.501524
Ag	1.197764	-0.613732	2.830077
Ag	4.163250	-1.054791	-1.851616
Ag	-0.412487	-0.433522	5.092362
Ag	-3.949010	-3.297107	-1.756169
Ag	2.263082	1.045369	-1.731728
Ag	-0.511088	0.171356	-1.789328
Ag	0.135851	2.874622	-1.454949
Ag	-3.231849	-0.660601	-1.694958
Ag	-2.662267	2.000849	-1.456083
Ag	-2.016222	4.654793	-1.163481
Ag	0.680461	1.137079	0.673691
Ag	-1.428718	3.015705	0.959190
Ag	-0.917030	1.330617	3.036411
Ag	-2.211546	0.302426	0.744894
O	7.694784	-3.392631	-0.909626
O	5.420600	4.017752	-0.811900
O	6.163628	-2.014967	-1.834398
N	5.265796	1.291365	0.667131
N	6.128382	-0.682170	0.720032
C	4.927241	-0.030613	0.746613
C	7.180692	0.215250	0.611731
H	8.208486	-0.119237	0.530200
C	6.636329	1.463432	0.581527
H	7.070811	2.447326	0.448556
C	4.306822	2.399584	0.572992
H	3.313554	1.923504	0.556217
C	4.551430	3.123809	-0.801278
C	6.360968	-2.126083	0.608605
H	7.235688	-2.343747	1.238504
C	6.785317	-2.548240	-0.849906
O	3.865480	2.703923	-1.793578
C	5.184163	-2.966425	1.082745
H	4.858454	-2.679789	2.093012
C	4.412069	3.332732	1.768112
H	3.607233	4.079014	1.714583
H	5.495010	-4.020088	1.085469
H	4.321749	-2.868560	0.404433
H	5.369821	3.870187	1.749627
H	4.307679	2.771713	2.708830

$[Ag_{20}(NHC^{iPr})]^{2-}$ face

Ag	-1.057235	0.000029	-1.849730

Ag	-3.368365	1.526153	-1.502920
Ag	1.354955	1.330443	-2.007379
Ag	-0.928101	-2.931772	-1.708372
Ag	-0.928215	2.931784	-1.708329
Ag	-3.368279	-1.526240	-1.502929
Ag	1.354984	-1.330342	-2.007369
Ag	1.709033	4.019797	-1.762538
Ag	1.709191	-4.019686	-1.762632
Ag	-5.705243	-0.000107	-1.267716
Ag	0.833657	2.753279	0.480557
Ag	-1.583413	1.455251	0.645930
Ag	0.329326	1.384927	2.723395
Ag	-3.993558	-0.000100	0.875755
Ag	-2.214055	-0.000076	2.976372
Ag	-0.375902	-0.000060	5.026951
Ag	1.838607	0.000001	0.611468
Ag	0.329402	-1.385029	2.723410
Ag	0.833767	-2.753325	0.480532
Ag	-1.583228	-1.455161	0.645857
O	3.947932	-4.321334	-1.663974
O	6.038103	3.529793	-1.422592
O	6.038257	-3.529573	-1.422697
N	4.709393	1.079840	-0.393700
N	4.709450	-1.079673	-0.393726
C	3.942744	0.000059	-0.049137
C	5.923776	-0.681885	-0.933294
H	6.634990	-1.423333	-1.276717
C	5.923794	0.682131	-0.933157
H	6.635019	1.423629	-1.276450
C	4.289039	2.466257	-0.137283
H	3.190162	2.440366	-0.219070
C	4.815831	3.505143	-1.180755
C	4.289187	-2.466123	-0.137338
C	4.613973	-2.872722	1.320895
C	4.815979	-3.504925	-1.180892
O	3.947760	4.321522	-1.663845
H	3.190305	-2.440290	-0.219053
C	4.613695	2.872805	1.320990
C	4.003632	4.238536	1.637380
H	4.095343	2.117387	1.940213
C	6.105658	2.831212	1.654926
C	4.004050	-4.238523	1.637257
C	6.105955	-2.831023	1.654729
H	4.095600	-2.117379	1.940191
H	4.154013	-4.488400	2.698744
H	2.918757	-4.241365	1.438220
H	4.456563	-5.030372	1.021911
H	6.259165	-3.085251	2.715539
H	6.665167	-3.543181	1.031519
H	6.528519	-1.830763	1.482093
H	4.153500	4.488372	2.698890
H	4.456122	5.030456	1.022106
H	2.918354	4.241294	1.438268
H	6.258772	3.085394	2.715761
H	6.528317	1.830997	1.482265
H	6.664852	3.543451	1.031794

$[Ag_{20}(NHC^{iPr})]^{2-}$ vertex

Ag	-2.856374	-0.097510	-0.225610
Ag	-2.671474	-2.908188	-0.174289
Ag	-3.042668	1.338274	2.188857
Ag	-2.463823	1.284520	-2.644583
Ag	-3.011376	-1.557862	2.178607
Ag	-2.328450	-1.435853	-2.645762
Ag	-2.838010	2.714402	-0.154009
Ag	-3.356822	-0.133447	4.488664
Ag	-2.578442	4.036608	-2.557382
Ag	-2.309221	-4.185436	-2.568534
Ag	-0.782921	-0.027721	3.306773
Ag	-0.462472	-1.520014	0.940414
Ag	1.676520	0.035075	1.965688
Ag	-0.073674	-2.809528	-1.535877
Ag	2.020403	-1.355837	-0.419012

Ag	4.136906	0.036800	0.692869
Ag	-0.493580	1.465398	0.916009
Ag	1.978702	1.621372	-0.493417
Ag	-0.293478	2.828577	-1.529268
Ag	-0.117559	0.027673	-1.585773
O	4.103128	2.154587	-1.669778
O	9.258772	-2.601940	0.090902
O	3.884213	3.086433	0.371477
N	7.123492	-0.619862	-0.031449
N	6.706999	1.443422	-0.506047
C	6.168099	0.342682	0.093250
C	7.975146	1.163550	-0.993973
H	8.572066	1.911479	-1.503515
C	8.236728	-0.143758	-0.702496
H	9.077818	-0.817540	-0.849539
C	6.918802	-2.007806	0.443936
H	6.329485	-1.909432	1.365936
C	8.243157	-2.790053	0.819302
C	6.117114	2.789498	-0.553994
C	6.716958	3.689931	0.549896
C	4.562208	2.679834	-0.616056
O	8.095609	-3.569185	1.789098
H	6.416773	3.207388	-1.529418
C	6.058587	-2.783528	-0.584678
C	5.542419	-4.091348	0.016258
H	5.179162	-2.136064	-0.781734
C	6.779716	-3.016547	-1.913314
H	4.892431	-4.609176	-0.706406
H	6.375698	-4.751443	0.295165
H	4.956800	-3.899686	0.927450
H	6.110880	-3.531641	-2.620519
H	7.090913	-2.067340	-2.373643
H	7.683620	-3.624721	-1.763753
C	6.225548	5.130931	0.384198
C	6.483124	3.171588	1.970611
H	7.808819	3.681911	0.367204
H	7.005755	3.815440	2.695707
H	5.410111	3.168547	2.200261
H	6.862374	2.147261	2.090758
H	6.743755	5.798369	1.090079
H	6.412331	5.505093	-0.635621
H	5.145591	5.184360	0.577650

$[Ag_{20}(NHC^{iPr})]^{2-}$ edge

Ag	-2.333398	-0.722574	-0.787022
Ag	-3.665322	-0.214433	1.654211
Ag	-2.131834	1.285422	-2.734505
Ag	-0.772204	-3.069309	-1.065254
Ag	-3.658397	1.717597	-0.286789
Ag	-2.155266	-2.665780	1.253457
Ag	-0.727652	-1.045121	-3.089147
Ag	-3.567240	3.624670	-2.237431
Ag	0.555767	-3.443517	-3.429750
Ag	-3.607196	-2.178312	3.555533
Ag	-1.185511	3.203593	-0.817743
Ag	-1.329292	1.316870	1.269766
Ag	1.068993	2.673658	0.685284
Ag	-1.208033	-0.753836	3.176168
Ag	1.098651	0.713761	2.666966
Ag	3.373855	2.137191	2.120218
Ag	0.304974	0.804949	-1.266637
Ag	2.681815	0.232181	0.208975
Ag	1.734122	-1.636016	-1.613653
Ag	0.216098	-1.155319	0.756733
O	3.608696	-2.921486	-1.847696
O	5.449530	2.838018	1.938640
O	5.370731	-4.269023	-1.438639
N	5.868934	0.616202	-0.196052
N	5.400655	-1.451788	0.189746
C	4.816014	-0.222715	0.050029

C	6.775557	-1.377131	0.032926
H	7.397171	-2.263746	0.062410
C	7.072094	-0.072195	-0.206023
H	8.015844	0.441210	-0.345734
C	5.871388	2.081182	-0.370540
H	6.715731	2.278407	-1.049316
C	6.298157	2.777313	0.978229
C	4.752313	-2.771408	0.317649
H	5.514925	-3.411556	0.787963
C	4.552902	-3.384460	-1.123010
O	7.460714	3.216545	1.006853
C	3.515554	-2.784857	1.214685
H	2.763018	-2.106098	0.766457
C	3.819119	-2.288186	2.628166
H	4.533198	-2.960120	3.134346
H	4.241120	-1.273650	2.620626
H	2.895386	-2.255001	3.225212
C	2.894544	-4.181956	1.230620
H	1.984286	-4.180233	1.847972
H	2.616235	-4.503704	0.217667
H	3.596206	-4.923332	1.648261
C	4.612208	2.639028	-1.037624
H	3.741777	2.395749	-0.397147
C	4.701065	4.163927	-1.116201
H	4.804471	4.609679	-0.117297
H	5.566476	4.478166	-1.722949
H	3.790451	4.568757	-1.581572
C	4.373861	2.024291	-2.417949
H	4.288983	0.930314	-2.369531
H	3.436343	2.407007	-2.847591
H	5.197612	2.280946	-3.105594

$[Ag_{30}(NHC^{H})]^{2-}$

Ag	-4.241355	-0.248373	0.053391
Ag	-3.409758	-0.169085	2.863510
Ag	-3.565102	-2.623192	1.658968
Ag	-2.650779	1.995674	1.282554
Ag	-0.038877	3.192985	1.489821
Ag	1.144384	0.509892	1.051961
Ag	-1.535534	-0.732259	0.698282
Ag	1.817873	2.029517	3.263444
Ag	-1.202671	-2.087198	3.136470
Ag	3.031609	-1.430745	-0.182156
Ag	3.877275	0.809115	1.481305
Ag	2.664469	3.232583	0.864570
Ag	1.406886	-0.825119	3.625668
Ag	0.839568	-2.304328	1.346403
Ag	-0.782027	0.824157	3.085254
Ag	-1.333964	-3.751462	0.426144
Ag	-1.172127	-3.091485	-2.302613
Ag	0.556564	-0.907693	-1.268869
Ag	2.706576	-0.750815	-3.121553
Ag	-3.597918	-2.749749	-1.075245
Ag	-0.087006	-1.087064	-3.890767
Ag	-0.758508	1.517945	-0.787117
Ag	2.813909	1.309074	-1.115392
Ag	-3.445842	2.013950	-1.415371
Ag	0.936220	1.421080	-3.110435
Ag	-1.267930	3.126753	-3.000293
Ag	0.981271	3.673039	-1.291639
Ag	-1.784926	4.148853	-0.432571
Ag	-2.261688	-0.488625	-2.116195
Ag	1.234843	-3.629477	-0.986434
O	4.488419	-1.956482	-3.714654
O	5.005153	-0.511716	3.030450
O	6.410445	-3.061831	-3.272086
N	5.593972	-2.565295	1.265507
N	6.102378	-1.744982	-0.661683
C	5.048654	-1.977237	0.165876
C	7.285095	-2.188920	-0.099223
H	8.228158	-2.133597	-0.628274
C	6.965845	-2.693517	1.129683
H	7.588320	-3.118335	1.908064
C	4.814145	-2.855374	2.456160

H	3.888650	-3.363509	2.151540
C	4.406776	-1.594445	3.277458
C	5.951924	-1.119960	-1.967967
H	5.184795	-0.337374	-1.867399
C	5.586323	-2.154042	-3.079586
O	3.489110	-1.812836	4.119844
H	6.910837	-0.654433	-2.235744
H	5.384649	-3.537181	3.102292

$[Ag_{30}(NHC^{Me})]^{2-}$

Ag	4.327428	-0.557935	0.237681
Ag	3.578558	-1.160177	-2.532723
Ag	3.472348	-3.210236	-0.719081
Ag	2.982956	1.403305	-1.617941
Ag	0.497884	2.713858	-2.259674
Ag	-0.934849	0.350306	-1.186670
Ag	1.606609	-0.970294	-0.391793
Ag	-1.411800	1.274842	-3.752170
Ag	1.210598	-2.891788	-2.401795
Ag	-3.022217	-1.030671	0.422248
Ag	-3.615378	0.739982	-1.819218
Ag	-2.206898	3.136710	-1.800760
Ag	-1.258853	-1.591486	-3.325248
Ag	-0.885554	-2.458717	-0.714086
Ag	1.060898	-0.048495	-3.138113
Ag	1.120443	-3.782881	0.660030
Ag	0.953628	-2.407779	3.107513
Ag	-0.536670	-0.444594	1.449514
Ag	-2.708341	0.376484	3.088660
Ag	3.429205	-2.607972	1.950619
Ag	0.018130	0.030985	4.053948
Ag	1.004483	1.651082	0.411766
Ag	-2.576604	1.834387	0.606616
Ag	3.709325	2.072942	1.015889
Ag	-0.748436	2.315954	2.592871
Ag	1.602522	3.746170	2.142568
Ag	-0.541731	3.997221	0.240662
Ag	2.279476	3.997229	-0.574327
Ag	2.283537	-0.048110	2.292353
Ag	-1.461132	-3.075605	1.863820
O	-4.641944	-0.441119	3.850697
O	-4.834015	-0.878269	-2.979860
O	-6.772767	-1.167370	3.661528
N	-5.669011	-2.271173	-0.761648
N	-6.118800	-0.843686	0.795743
C	-5.084557	-1.433387	0.138141
C	-7.332806	-1.311557	0.326241
H	-8.278130	-0.999585	0.749714
C	-7.049491	-2.202365	-0.670206
H	-7.709988	-2.778686	-1.304823
C	-4.877562	-2.984398	-1.764413
H	-3.985628	-3.353462	-1.233276
C	-4.326432	-2.027869	-2.876813
C	-5.907075	0.145775	1.857454
H	-4.951750	0.633164	1.601303
C	-5.768255	-0.565060	3.248512
O	-3.393538	-2.539566	-3.563116
C	-7.018784	1.182302	1.892757
H	-7.179992	1.628634	0.900156
C	-5.625922	-4.159367	-2.379885
H	-6.492218	-3.822519	-2.969297
H	-7.951581	0.732748	2.261697
H	-6.732114	1.981051	2.590449
H	-5.971744	-4.864526	-1.609593
H	-4.938713	-4.678368	-3.058718

$[Ag_{30}(NHC^{iPr})]^{2-}$

Ag	4.425711	-0.619742	0.411736
Ag	3.662985	-1.841217	-2.140488
Ag	3.476587	-3.391526	0.108763
Ag	3.165879	0.887565	-1.872278

Ag	0.726140	2.088151	-2.835354
Ag	-0.795456	0.089960	-1.244755
Ag	1.691154	-1.075128	-0.123766
Ag	-1.235987	0.411125	-3.958293
Ag	1.238157	-3.403519	-1.631675
Ag	-2.932277	-0.806375	0.635738
Ag	-3.462868	0.441543	-1.970921
Ag	-1.957979	2.716492	-2.517378
Ag	-1.171033	-2.281511	-2.863703
Ag	-0.844887	-2.525541	-0.115501
Ag	1.195843	-0.810572	-3.023803
Ag	1.107583	-3.544766	1.564742
Ag	0.980152	-1.605791	3.600592
Ag	-0.443301	-0.045881	1.514078
Ag	-2.562920	1.269387	2.892180
Ag	3.450941	-2.165629	2.556890
Ag	0.134462	1.023254	3.929295
Ag	1.184725	1.681601	0.015696
Ag	-2.352403	2.021829	0.126016
Ag	3.903722	2.141528	0.530438
Ag	-0.520804	2.931219	1.958661
Ag	1.878121	4.116753	1.192065
Ag	-0.261650	3.979675	-0.726506
Ag	2.552486	3.676285	-1.496301
Ag	2.395851	0.440535	2.261130
Ag	-1.446241	-2.485181	2.527704
O	-4.586552	0.869968	3.750566
O	-4.768963	-1.290701	-2.900042
O	-6.552092	-0.228222	3.549481
N	-5.628968	-2.038611	-0.451707
N	-6.000414	-0.271622	0.738675
C	-5.012065	-1.118199	0.337434
C	-7.216595	-0.652073	0.202919
H	-8.139520	-0.128446	0.410731
C	-6.979520	-1.756086	-0.565932
H	-7.653893	-2.343374	-1.175502
C	-4.868236	-3.033757	-1.210749
H	-3.979380	-3.251491	-0.593365
C	-4.295599	-2.399255	-2.527189
C	-5.690207	0.874568	1.597858
H	-4.677784	1.173028	1.274117
C	-5.610852	0.442755	3.100046
O	-3.360037	-3.062278	-3.065462
C	-6.608909	2.092046	1.362615
H	-6.841859	2.095898	0.282004
C	-5.664145	-4.343014	-1.389170
H	-6.567454	-4.114446	-1.985003
C	-5.823461	3.371121	1.677125
H	-5.484986	3.366755	2.723906
H	-4.929371	3.456861	1.040577
H	-6.451261	4.261498	1.518330
C	-7.925103	2.076760	2.150822
H	-8.558259	2.919921	1.831471
H	-8.489742	1.143470	2.029524
H	-7.728820	2.176721	3.227625
C	-4.865764	-5.408798	-2.145257
H	-5.464545	-6.330426	-2.221065
H	-4.579792	-5.076072	-3.148813
H	-3.935463	-5.646909	-1.607747
C	-6.098898	-4.894285	-0.024348
H	-5.212520	-5.133277	0.583866
H	-6.708996	-4.180913	0.545235
H	-6.679947	-5.820563	-0.153110