Supporting Information for:

Insight into the Nature of Carbon-Metal Bonding of *N*-Heterocyclic Carbenes in Gold/Silver Complexes and Nanoparticles Using DFT-Correlated Raman Spectroscopy: Strong Evidence for π-Backbonding.

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I. General Procedure

Synthesis of compound 2:

One equivalent (0.8 M) of the benzimidazole (**1**) was dissolved in DMSO with a stir bar in a round bottom flask. The crushed base (KOH, 1.5 equivalent) was then added to the mixture and the reaction was stirred for 2 h at room temperature. Drop by drop, the bromododecane (1.2 equivalent) was added and the reaction was left running at room temperature for 24 hours.

^{1}H NMR ($CDCl_3$, 300 MHz): δ (ppm) = 7.88 (s, 1H, carbonic H), 7.79 (m, 1H, aromatic H), 7.38 (m, 1H, aromatic H), 7.26 (m, 2H, aromatic H), 4.17 (t, *J* = 7.2 Hz, 2H, alkyl H), 1.88 (t, *J* = 6.9 Hz, 2H, alkyl H), 1.31 (m, 18H, alkyl H), 0.88 (m, 3H, alkyl H).

Synthesis of compound 3:

The compound **2** (1 equivalent, 2M) was dissolved in ACN with a stir bar in a pressure tube. In liquid form, 10 equivalent of the bromododecane was added to the mixture. The pressure tube was then closed and heated to 90°C for 24 hours. The ACN was then removed with a rotary evaporator. To remove the impurities, hexane was added before sonicating and centrifuging. The hexane layer was removed, and this process was repeated 6 times.

^{1}H NMR ($CDCl_3$, 300 MHz): δ (ppm) = 11.33 (s, 1H, carbenic H), 7.69 (m, 2H, aromatic H), 7.64 (m, 2H, aromatic H), 4.60 (t, *J* = 5.6 Hz, 4H, alkyl H), 2.01 (t, *J* = 5.4 Hz, H, alkyl H), 1.19 (m, 36H, alkyl H), 0.82 (m, 6H, alkyl H).

Synthesis of C_{12}NHC-AuBr:

Compound **3** (100 mg, 0.23 mmol) was dissolved in ACN (10 mL) in a 25 mL round bottom flask. The solution was stirred before adding Me_2SAuCl (99.8 mg, 400 mmol) and crushed K_2CO3 (94 mg, 678 mmol). The reaction was stirred at 62°C overnight (12h). After cooling the reaction at room temperature, the mixture was filtered through celite and washed twice with cold diethyl ether. The compound formed was purified by column chromatography using DCM as initial eluent to remove the impurities before switching eluant to MeOH/DCM (10%) to recover the product. The solvent was removed with a rotary evaporator (out of the bath) to recover 88.5 mg of a white (lightly yellow) powder (55% yield).

^{1}H NMR ($CDCl_3$, 300 MHz): δ (ppm) = 7.45 (m, 4H, aromatic H), 4.47 (t, *J* = 6.0 Hz, 4H, alkyl H), 1.94 (m, 4H, alkyl H), 1.35 (m, 36H, alkyl H), 0.87 (t, *J* = 6.5 Hz, 6H, alkyl H).

^{13}C NMR (DMSO, 300 MHz): δ (ppm) = 181.22, 133.06, 124.35, 111.53, 48.83, 31.91, 29.61 (6), 26.76, 22.69 and 14.23.

Synthesis of C_{12}NHC-AuNP:

The **C_{12}NHC-AuNPs** were obtained by dissolving **C_{12}NHC-AuBr** (18 mg, 25 µmol) in DCM (885 µL) with a stir bar in a round bottom flask. A solution of tert-butylamine borane was prepared by dissolving 22 mg (249 µmol) of this compound in DCM (885 µL). This solution was added to the DCM solution of the complex and the mixture was stirred for 24 h at room temperature. The nanopartiles were purified by precipitation with cold diethyl ether and then washed 3 times with the same cold solvent. After extracting the solvent, the pure gold nanoparticles formed a light red powder (13 mg) and were stabilized and kept in a vial with THF.

UV-Vis spectroscopy: Surface Plasmon Resonance at 526 nm (see Figure S17.)

Synthesis of $[(C_{12}NHC)_2\text{-}Ag]^+$ $[AgBr_2]^-$:

The quaternary compound **3** (50 mg, 113 mmol) was dissolved in ACN (15 mL) with a stir bar in a 25 mL round bottom flask wrapped in aluminum foil. In a darkened room, 131 mg (565 mmol) of silver oxide (Ag2O) was added as a solid in the round bottom flask. The reaction was stirred for 3 h at room temperature. The complex formed was purified by filtration through celite (with additional DCM for rinsing) followed by filtration through cotton. The solvent was then removed by blowing air in the round bottom flask to recover 102.6 mg of off-white powder (35% yield).

^{1}H NMR ($CDCl_3$, 300 MHz): δ (ppm) = 7.46 (m, 2H, aromatic H), 7.42 (m, 2H, aromatic H), 4.38 (t, *J* = 7.2 Hz, 4H, alkyl H), 1.90 (t, *J* = 6.8 Hz, 4H, alkyl H), 1.31 (m, 36H, alkyl H), 0.87 (t, *J* = 6.4 Hz, 6H, alkyl H).

^{13}C NMR (DMSO, 300 MHz): δ (ppm) = 133.79, 124.08, 111.64, 49.73, 32.02, 30.50, 29.71 (5), 27.00, 22.80, 14.23.

Synthesis of C_{12}NHC-AgNP:

The NHC-functionalized AgNPs (**C_{12}NHC-AgNP**) were obtained by dissolving **bis-C_{12}NHC-Ag^+ $AgBr_2^-$** (69 mg, 0.11 mmol) in toluene (40 mL) with a stir bar in a 100 mL round bottom flask wrapped in aluminum foil. A solution of tert-butylamine borane was prepared by dissolving 48 mg (5.5 mmol) of this compound in toluene (10 mL). This solution was then added to the toluene solution of 6 and was stirred overnight (for 12 h) at room temperature. After the reaction, the solvent was removed by blowing air in the round bottom flask wrapped in aluminum foil. The dried AgNPs were quickly redissolved in THF (5 mL). Residual small molecule impurities were removed by placing the AgNPs solution in a 12-14K molecular weight cut-off (MWCO) membrane which was dialysed in sequential baths of THF in the absence of light. The pure nanoparticles (inside the membrane) were placed in a vial (wrapped in aluminum foil) and kept in solution. The calculated mass of the off-white nanoparticle solution was 41.4 mg.
UV-Vis spectroscopy: Surface Plasmon Resonance at 423 nm (see Figure S18.)

Synthesis of compound 4:

In a 50 mL round bottom flask with a stir bar, 960 mg (8.1 mmol) of benzimidazole (**1**) with 98 mg (24.4 mmol) of NaOH were dissolved in DMSO (20 mL). The mixture was stirred in a closed system at 70°C for 2h before adding 739 µL of 1-bromopropane. The reaction was then stirred for 12 h at 100°C. The mixture was added into a separating funnel with cold DI-water. The aqueous phase was extracted 3 times with DCM before adding $MgSO_4$ to dry our phase followed by filtration. The DCM was removed with a rotary evaporator and the DMSO was removed by extraction with hexane: diethyl ether (1:1) 3 times before adding $MgSO_4$ and filtering the solution. The solvent was then removed with a rotary evaporator to recover 1.10 g of red-orange powder (85% yield).
^{1}H NMR ($CDCl_3$, 300 MHz): δ (ppm) = 7.96 (s, 1H, carbenic H), 7.81 (m, 1H, aromatic H), 7.39 (m, 1H, aromatic H), 7.32 (m, 2H, aromatic H), 4.15 (t, J = 7.8 Hz, 2H, alkyl H), 1.91 (sept, J = 7.4 Hz, 2H, alkyl H), 0.96 (t, J = 7.1 Hz, 3H, alkyl H).

Synthesis of compound 5:

The quaternary product **5** was obtained by dissolving the compound **4** (320 mg, 2.0 mmol) with 1.23 g (2.00 mmol) of 1-bromopropane in ACN (6.4 mL) in a 25 mL pressure tube equipped with a stir bar. The reaction was stirred overnight (12 h) at 100°C. The compound formed was purified by column chromatography first using EtOAc and switching eluant to MeOH/EtOAc (10%) to collect the product. The solvent was removed with a rotary evaporator to recover 479 mg of a dark red-orange powder (85% yield).
^{1}H NMR ($CDCl_3$, 300 MHz): δ (ppm) = 11.48 (s, 1H, carbenic H), 7.71 (m, 4H, aromatic H), 4.61 (t, J = 7.3 Hz, 4H, alkyl H), 2.10 (sept, J = 7.4 Hz, 4H, alkyl H), 1.05 (t, J = 7.4 Hz, 6H, alkyl H)

Synthesis of C_3NHC-AuBr:

The quaternary compound **5** (100 mg, 0.354 mmol) and Chloro(dimethyl sulfide)gold(I) (125 mg, 0.424 mmol) were dissolved in acetone (10 mL) with a stir bar in a 25 mL pressure tube. Crushed potassium carbonate (146 mg, 1.06 mmol) was added before closing the pressure tube and letting the reaction stirred overnight at 60°C. The complex formed was purified by filtration through celite (with additional acetone for rinsing) followed by removing the solvent with a rotary evaporator. The compound formed dissolved with minimum DCM and purified by column chromatography using DCM as eluent to recover the product. The DCM was removed with a rotary evaporator (out of the bath) to recover 146.0 mg of a light-yellow powder (86% yield).
^{1}H NMR ($CDCl_3$, 300 MHz): δ (ppm) = 7.46 (m, 2H, aromatic H), 7.38 (m, 2H, aromatic H), 4.40 (t, J = 7.4 Hz, 4H, alkyl H), 1.93 (sept, J = 7.4 Hz, 4H, alkyl H), 0.95 (t, J = 7.5 Hz, 6H, alkyl H).
^{13}C NMR (DMSO, 300 MHz): δ (ppm) = 180.80, 132.97, 124.44, 111.60, 50.43, 23.26 and 11.20.

Synthesis of C_3NHC-AuNP:

The **C_3NHC-AuNPs** were obtained by dissolving complex 10 (30 mg, 6.26 mmol) in DCM (12 mL) with a stir bar in a 25 mL round bottom flask. A solution of sodium borohydride ($NaBH_4$) was prepared by dissolving 24 mg (6.26 mmol) of this compound in DI-water (12 mL). The $NaBH_4$ solution was then added to the DCM solution containing compound 10 and the biphasic mixture was stirred for 1h at room temperature. The organic phase was extracted with DI-water and the organic phase was dried using a stream of air. The gold nanoparticles were purified by precipitation with cold THF and washed 3 times with cold THF.
After extracting the THF, the pure nanoparticles formed a purple powder (139 mg) and were stabilized and kept in a vial with DCM.
UV-Vis spectroscopy: Surface Plasmon Resonance at 552 nm (see Figure S19)

II. DFT Data

1.1. Computational protocol for modelling the Raman spectrum of complexes and nanoparticles.

1- Model several possible conformers of a single molecule of your complex in a modelling software (ex: Avogadro, GaussView or ChemCraft) and export each set of cartesian atomic coordinates to a .xyz file.

2- Optimized each conformer of the complex with ORCA at the r²SCAN-3c level of theory in gas phase. An example input file can be used from *section 2.1*. The pre-optimized molecules are ranked by their final single point energies (SPE), and the three most stable conformers are selected.

3- For nanoparticles, repeat *1* and *2* for the ligand only. Again, with Avogadro, put in different input files the three stable pre-optimized ligands with the metallic cluster and calculate the Raman spectrum for each three nanoparticles (see *4*).

4- For each of the three pre-optimized complexes, we calculate the Raman spectrum with ORCA at the r²SCAN-3c level of theory in gas phase, with the TightOpt and TightSCF commands (example input in *section 2.2*). When a spectrum without imaginary frequencies in an ORCA output file is obtained, the spectral information can be obtained from the output file.

5- The software ChemCraft can read an ORCA output to visualize (and extract) the optimized molecule with its Raman vibrations.

1.2. ORCA Input file example for pre-optimization

```
# [MOLECULE IDENTIFIER]
!Opt r2SCAN-3c

%pal
    nprocs 16 # Number of cores
end

%maxcore 3000 # Memory allocation per core

*xyz 0 1 # Charge and multiplicity
 [CARTESIAN ATOMIC COORDINATES HERE]
*
```

1.3. ORCA Input file example for final frequency calculation

```
# [MOLECULE IDENTIFIER]
!Opt NumFreq r2SCAN-3c TIGHTOPT

%elprop
    polar 1 # Calculate Raman spectrum
end

%pal
    nprocs 16 # Number of cores
end

%maxcore 3000 # Memory allocation per core

*xyz 0 1 # Charge and multiplicity
 [DIMER CARTESIAN ATOMIC COORDINATES HERE]
*
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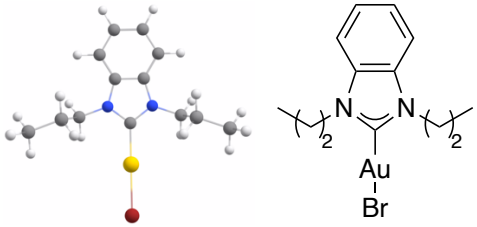
1.4. Optimized atomic coordinates



Name: **C_3NHC-AuBr**

Qty of imaginary frequencies: 0

Final single point energy (Eh): -3325.37445244

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N	-1.365311	-1.030049	1.699887
C	-0.360972	-0.903850	0.791094
C	-2.307836	-0.328111	-0.197824
C	-3.315766	0.074967	-1.065252
C	-2.584726	-0.698057	1.127002
C	-4.611822	0.094090	-0.560344
H	-3.107989	0.358501	-2.091789
C	-3.879462	-0.678648	1.631201
C	-4.888422	-0.275903	0.762425
H	-5.427575	0.400518	-1.207174
H	-4.099670	-0.968085	2.653445
H	-5.913640	-0.249702	1.117313
Au	1.554828	-1.365181	1.064295
Br	3.874572	-1.963461	1.384211
C	-1.183616	-1.559469	3.049793
H	-1.887410	-1.043065	3.714646
H	-0.167006	-1.297805	3.364296
C	-1.382566	-3.072350	3.104771
H	-0.660818	-3.536579	2.421052
H	-2.385407	-3.322880	2.735126
C	-1.185990	-3.603000	4.521742
H	-1.902295	-3.154360	5.219495
H	-1.322054	-4.687321	4.554649
H	-0.176676	-3.382450	4.885520
C	-0.210482	-0.257792	-1.611230
H	0.821404	-0.000335	-1.347061
H	-0.653494	0.603508	-2.127003
C	-0.237453	-1.502700	-2.494637
H	-1.278581	-1.778310	-2.707293
H	0.207389	-2.332184	-1.930865
C	0.530419	-1.272559	-3.792944
H	0.095983	-0.450517	-4.373178
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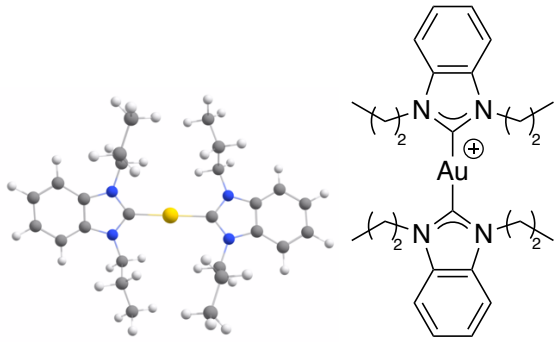

Name: **[$(C_3NHC)_2$-Au]$^+$**

Qty of imaginary frequencies: 0

Final single point energy (Eh): -1366.33547980

Au	2.200130000	-0.062103000	19.299195000
N	-0.194260000	1.809655000	19.117633000
N	-0.728831000	-0.201733000	18.479377000
C	0.288264000	0.552544000	18.962842000
C	-1.519792000	1.873773000	18.704515000
C	-1.863990000	0.578248000	18.294392000
C	-0.611531000	-1.610458000	18.105376000
H	0.175809000	-2.048142000	18.730640000
H	-1.553957000	-2.109039000	18.362905000
C	0.607382000	2.951548000	19.554864000
H	1.370765000	2.571081000	20.243649000
H	-0.044187000	3.624335000	20.124646000
C	1.257885000	3.682312000	18.382138000
H	1.894943000	2.969021000	17.840898000
H	0.480688000	4.007398000	17.679475000
C	2.075733000	4.878275000	18.860391000
H	2.873775000	4.567575000	19.544634000
H	1.448321000	5.603217000	19.389948000
C	-0.179088000	-3.269001000	16.260333000
H	-1.126273000	-3.790390000	16.435905000
H	0.593695000	-3.771193000	16.853302000
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H	-1.049153000	-1.299006000	16.017606000
H	0.667258000	-1.277955000	16.417130000
C	-2.435555000	2.919342000	18.660832000
H	-2.178272000	3.925469000	18.974691000
C	-3.137042000	0.275717000	17.823824000
H	-3.410293000	-0.723882000	17.502632000
C	-3.706517000	2.617253000	18.189599000
H	-4.452109000	3.403684000	18.136879000
C	-4.050827000	1.320406000	17.779106000
H	-5.055687000	1.129795000	17.416992000
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N	5.241437000	0.057628000	19.439933000
C	4.117159000	-0.685639000	19.583082000
C	5.902635000	-2.021726000	19.911974000
C	6.370192000	-0.731882000	19.625053000
C	5.260973000	1.466272000	19.049350000
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H	6.080268000	1.955618000	19.590067000
C	3.607315000	-3.076333000	20.071022000
H	2.667302000	-2.677488000	20.469911000
H	4.037275000	-3.733033000	20.836688000
C	3.359138000	-3.839621000	18.771811000
H	2.938913000	-3.142092000	18.034047000
H	4.316067000	-4.189560000	18.365200000
C	2.415033000	-5.017352000	18.995065000
H	1.442870000	-4.682740000	19.375389000
H	2.828185000	-5.727385000	19.719424000
C	5.454747000	3.126922000	17.166472000
H	6.308851000	3.632042000	17.630270000
H	4.544305000	3.643103000	17.491351000
C	5.412232000	1.648628000	17.540976000

H	6.324087000	1.141822000	17.201641000
H	4.568780000	1.150736000	17.044897000
C	6.775347000	-3.074530000	20.164083000
H	6.422131000	-4.076220000	20.385145000
C	7.729440000	-0.442264000	19.578718000
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C	8.132752000	-2.785399000	20.116221000
H	8.849691000	-3.577615000	20.304898000
C	8.600829000	-1.494079000	19.829329000
H	9.670323000	-1.313498000	19.801882000
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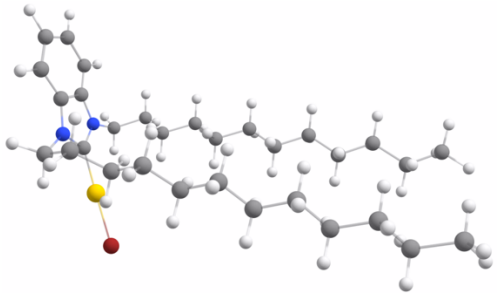

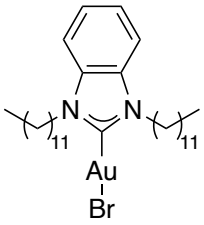

Name: **C_{12}NHC-AuBr**

Qty of imaginary frequencies: 0

Final single point energy (Eh): -4032.30255339

Au	1.993289000	-0.199773000	18.763671000
Br	4.224676000	-1.092501000	18.493571000
N	-0.189613000	1.852886000	19.081745000
N	-1.015374000	-0.158291000	18.914490000
C	0.152814000	0.541689000	18.947263000
C	-1.569870000	1.994067000	19.118155000
C	-2.100632000	0.700622000	19.011867000
C	-1.110530000	-1.590555000	18.635231000
H	-0.118552000	-2.010295000	18.835966000
H	-1.820295000	-2.033343000	19.345071000
C	0.752985000	2.971506000	19.064268000
H	1.728449000	2.569446000	19.360582000
H	0.432593000	3.689551000	19.828824000
C	0.835843000	3.629723000	17.684988000
H	-0.173191000	3.918769000	17.358412000
H	1.407682000	4.560810000	17.794268000
C	1.494576000	2.741635000	16.631924000
H	0.997149000	1.762577000	16.604714000
H	2.532095000	2.535585000	16.931354000
C	1.467847000	3.348300000	15.231041000
H	0.424423000	3.433930000	14.892360000
H	1.866441000	4.373199000	15.260254000
C	2.126739000	3.028733000	12.788009000
H	1.076033000	2.938139000	12.473458000
H	2.364147000	4.102467000	12.751612000
C	-0.991141000	-1.612549000	14.721711000
H	-0.966416000	-2.705831000	14.605619000
H	-2.032576000	-1.307730000	14.540210000
C	2.268007000	2.524838000	14.222516000
H	1.948635000	1.473544000	14.272262000
H	3.328017000	2.531536000	14.513193000
C	-0.597942000	-1.247893000	16.151554000
H	0.436725000	-1.563259000	16.349046000
H	-0.605562000	-0.153743000	16.258189000
C	-1.529837000	-1.868827000	17.190267000
H	-1.554003000	-2.959743000	17.065776000
H	-2.555782000	-1.513333000	17.023295000

C	-0.479582000	-1.358924000	12.242426000
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H	-1.508450000	-1.023438000	12.045513000
C	-0.086580000	-0.975063000	13.667960000
H	0.955228000	-1.272979000	13.854876000
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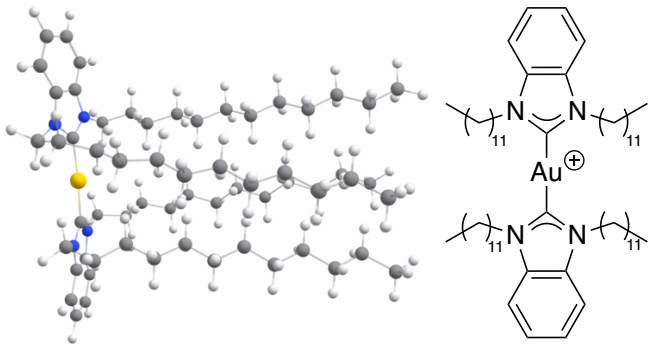
C	2.835798000	2.749690000	10.355475000
H	1.789897000	2.589806000	10.052165000
H	3.006781000	3.835001000	10.298667000
C	0.452480000	-0.789162000	11.174700000
H	1.477725000	-1.139103000	11.364516000
H	0.483498000	0.307692000	11.258807000
C	0.581701000	-1.078818000	7.266720000
H	0.460401000	-2.170638000	7.208782000
H	-0.408130000	-0.649836000	7.051945000
C	0.038592000	-1.180754000	9.756756000
H	-0.042859000	-2.275958000	9.694457000
H	-0.967559000	-0.787895000	9.549535000
C	3.760878000	2.040146000	9.368946000
H	3.587903000	0.955476000	9.426634000
H	4.806226000	2.200192000	9.670771000
C	3.573981000	2.505746000	7.926681000
H	2.525093000	2.354861000	7.629389000
H	3.754043000	3.589311000	7.865147000
C	1.006338000	-0.690326000	8.681953000
H	2.008358000	-1.095920000	8.885172000
H	1.101881000	0.403887000	8.746108000
C	3.019321000	2.282954000	11.797933000
H	2.813555000	1.204284000	11.861848000
H	4.071148000	2.410952000	12.091804000
C	-2.390483000	3.107990000	19.249761000
H	-1.985097000	4.111129000	19.330334000
C	-3.471745000	0.473534000	19.037449000
H	-3.887301000	-0.525698000	18.961934000
C	-3.762670000	2.881039000	19.271556000
H	-4.437441000	3.725134000	19.371478000
C	-4.293193000	1.588379000	19.168469000
H	-5.369748000	1.453185000	19.191798000
C	1.134164000	-0.992101000	4.780894000
H	1.862209000	-0.655150000	4.035731000
H	0.168906000	-0.533870000	4.537223000
H	1.022332000	-2.076952000	4.672962000
C	1.572344000	-0.624573000	6.196403000
H	2.556192000	-1.066791000	6.405412000
H	1.706770000	0.463217000	6.269631000
C	4.486424000	1.784270000	6.936272000
H	5.533539000	1.940030000	7.230482000
H	4.305948000	0.702851000	7.005286000
C	4.283426000	2.247197000	5.495465000
H	3.250669000	2.076383000	5.169913000
H	4.943454000	1.713234000	4.804112000
H	4.488413000	3.319102000	5.394069000



Name: **[(C_{12}NHC)$_2$-Au]$^+$**

Qty of imaginary frequencies: 0

Final single point energy (Eh): -2780.20602432

Au	2.216087000	-0.152419000	19.166772000
N	-0.266608000	1.577743000	18.951536000
N	-0.748268000	-0.491434000	18.467279000
C	0.264307000	0.334058000	18.827659000
C	-1.621568000	1.555817000	18.650476000
C	-1.935420000	0.222440000	18.350687000
C	-0.586457000	-1.914809000	18.165675000
H	0.431851000	-2.174863000	18.476341000
H	-1.286505000	-2.483130000	18.791296000
C	0.517992000	2.785495000	19.210043000
H	1.433571000	2.452936000	19.711390000
H	-0.037681000	3.413916000	19.915472000
C	0.861747000	3.548149000	17.925446000
H	-0.019611000	4.089691000	17.558955000
H	1.606280000	4.310493000	18.190862000
C	1.396431000	2.638469000	16.821360000
H	0.569394000	2.028875000	16.430364000
H	2.114531000	1.919027000	17.245431000
C	2.059894000	3.376797000	15.661801000
H	1.457719000	4.251668000	15.377905000
H	3.036502000	3.768965000	15.983118000
C	3.062633000	3.080198000	13.320955000
H	2.714623000	4.103994000	13.121046000
H	4.110390000	3.170413000	13.644593000
C	-0.170521000	-1.884213000	14.275088000
H	0.173233000	-2.924718000	14.177183000
H	-1.251800000	-1.905508000	14.073294000
C	2.230363000	2.469216000	14.445042000
H	1.233147000	2.214925000	14.057418000
H	2.680655000	1.512677000	14.754717000
C	0.048484000	-1.416001000	15.713884000
H	1.114842000	-1.481910000	15.979865000
H	-0.225650000	-0.354565000	15.796829000
C	-0.793854000	-2.240661000	16.686923000
H	-0.565971000	-3.308229000	16.565203000
H	-1.852851000	-2.127166000	16.423697000
C	0.184105000	-1.533537000	11.799363000
H	0.494866000	-2.585628000	11.712924000
H	-0.907639000	-1.531645000	11.664107000
C	0.507285000	-1.028981000	13.205942000
H	1.596347000	-1.022435000	13.361782000
H	0.174576000	0.014601000	13.305297000
C	3.873114000	2.798821000	10.912589000
H	3.651556000	3.863528000	10.748543000
H	4.927369000	2.750350000	11.222877000
C	0.827796000	-0.731373000	10.670731000
H	1.922527000	-0.760046000	10.774607000
H	0.539713000	0.326485000	10.758299000
C	0.691732000	-1.053240000	6.765056000
H	0.876228000	-2.137080000	6.721395000
H	-0.393724000	-0.926024000	6.640685000
C	0.430272000	-1.253488000	9.290224000
H	0.668339000	-2.326025000	9.227288000
H	-0.661235000	-1.179225000	9.176270000
C	3.691130000	2.037310000	9.602630000
H	2.640720000	2.109980000	9.285793000
H	3.876328000	0.965322000	9.773546000
C	4.595866000	2.532116000	8.477165000
H	4.409823000	3.601590000	8.300292000
H	5.647693000	2.452150000	8.790426000
C	1.112627000	-0.524698000	8.135056000
H	2.202990000	-0.619492000	8.241616000
H	0.891751000	0.551007000	8.195855000
C	2.985800000	2.264278000	12.033167000
H	1.941570000	2.243366000	11.689124000
H	3.250231000	1.216071000	12.242887000
C	-2.588320000	2.555168000	18.638506000
H	-2.350434000	3.588017000	18.869938000
C	-3.236069000	-0.166529000	18.047338000
H	-3.494198000	-1.198531000	17.837484000
C	-3.883901000	2.167521000	18.322354000
H	-4.670458000	2.914623000	18.302103000
C	-4.202088000	0.831514000	18.036902000
H	-5.229520000	0.570574000	17.805454000

C	1.009735000	-0.938745000	4.244303000
H	1.537853000	-0.438043000	3.426764000
H	-0.065556000	-0.815384000	4.073175000
H	1.234098000	-2.009781000	4.180969000
C	1.417356000	-0.375878000	5.603725000
H	2.501662000	-0.491420000	5.740730000
H	1.218489000	0.704553000	5.633207000
C	4.399068000	1.758988000	7.175546000
H	4.581875000	0.691987000	7.366574000
H	3.348620000	1.833468000	6.863323000
C	5.310068000	2.236387000	6.048595000
H	5.116837000	3.286509000	5.802812000
H	5.164225000	1.646385000	5.137848000
H	6.364549000	2.151250000	6.334984000
N	4.679995000	-1.783832000	19.933980000
N	5.166728000	0.330394000	19.735409000
C	4.158906000	-0.571764000	19.618726000
C	6.029874000	-1.664456000	20.242431000
C	6.341434000	-0.303766000	20.120979000
C	5.068758000	1.740733000	19.356646000
H	4.000146000	1.953880000	19.241295000
H	5.448227000	2.350570000	20.185977000
C	3.974088000	-3.059964000	19.812466000
H	2.901917000	-2.839993000	19.871330000
H	4.238814000	-3.675251000	20.680071000
C	4.318948000	-3.768932000	18.501750000
H	5.409286000	-3.883834000	18.434593000
H	3.903185000	-4.783550000	18.546576000
C	3.798880000	-3.045024000	17.260759000
H	4.055078000	-1.977306000	17.315015000
H	2.698874000	-3.091967000	17.246572000
C	4.362184000	-3.617906000	15.962878000
H	5.457619000	-3.520983000	15.980742000
H	4.151878000	-4.695684000	15.908881000
C	4.502993000	-3.417343000	13.435359000
H	5.581040000	-3.208677000	13.504530000
H	4.408282000	-4.510993000	13.368128000
C	6.186385000	1.567146000	15.608246000
H	5.931018000	2.603479000	15.342721000
H	7.265083000	1.565740000	15.823147000
C	3.818759000	-2.930905000	14.711161000
H	3.949971000	-1.841580000	14.804083000
H	2.734689000	-3.104812000	14.636876000
C	5.430844000	1.169301000	16.875108000
H	4.345616000	1.226875000	16.701457000
H	5.650698000	0.117704000	17.109820000
C	5.819525000	2.050995000	18.060713000
H	5.625804000	3.105340000	17.822340000
H	6.900871000	1.969940000	18.228268000
C	6.761203000	1.054782000	13.194047000
H	6.570012000	2.110747000	12.951461000
H	7.826631000	0.992543000	13.459490000
C	5.921685000	0.659744000	14.408100000
H	4.853990000	0.691663000	14.144014000
H	6.141796000	-0.383549000	14.681105000
C	4.650870000	-3.296091000	10.900869000
H	5.726885000	-3.077513000	10.970107000
H	4.563520000	-4.391622000	10.857758000
C	6.500900000	0.202669000	11.954380000
H	5.446008000	0.300903000	11.658756000
H	6.653615000	-0.859492000	12.198236000
C	8.008431000	0.159170000	8.336141000
H	7.886405000	1.230216000	8.115639000
H	9.061662000	0.025257000	8.623276000
C	7.392074000	0.588503000	10.774788000
H	7.260386000	1.659083000	10.558033000
H	8.446633000	0.462820000	11.060193000
C	4.098065000	-2.696382000	9.610924000
H	4.206562000	-1.601811000	9.645213000
H	3.017456000	-2.893580000	9.548526000
C	4.783271000	-3.231929000	8.355279000
H	5.862926000	-3.030957000	8.415251000
H	4.675106000	-4.325867000	8.318576000
C	7.109096000	-0.219607000	9.510899000
H	6.057369000	-0.080314000	9.219289000
H	7.226138000	-1.291442000	9.729295000

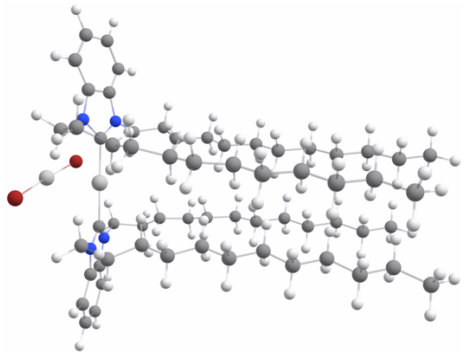
C	3.951106000	-2.786645000	12.159551000
H	4.052925000	-1.692357000	12.219545000
H	2.872683000	-2.991070000	12.085232000
C	6.982086000	-2.599707000	20.633181000
H	6.747444000	-3.654392000	20.730363000
C	7.616758000	0.178175000	20.398099000
H	7.863080000	1.231932000	20.325765000
C	8.257347000	-2.119267000	20.900690000
H	9.031162000	-2.814301000	21.209508000
C	8.567788000	-0.755857000	20.787962000
H	9.575014000	-0.422282000	21.014926000
C	8.618000000	-0.264467000	5.900356000
H	8.391865000	-0.859138000	5.009661000
H	9.674984000	-0.416742000	6.145708000
H	8.487149000	0.791365000	5.637699000
C	7.721972000	-0.652182000	7.073823000
H	6.667675000	-0.521069000	6.791078000
H	7.848647000	-1.720815000	7.297229000
C	4.231980000	-2.624612000	7.067740000
H	3.150320000	-2.810734000	7.012502000
H	4.348703000	-1.532935000	7.112124000
C	4.911864000	-3.158918000	5.810393000
H	5.988703000	-2.956407000	5.830920000
H	4.501659000	-2.695787000	4.906912000
H	4.778479000	-4.242806000	5.720834000

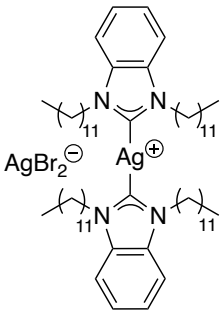
Main article molecule number: **$AgBr_2^-$**

Qty of imaginary frequencies: 0

Final single point energy (Eh): -5295.56376101

Ag	-0.577654000	0.853912000	0.000000000
Br	1.898891000	0.724902000	0.000000000
Br	-3.054200000	0.982914000	0.000000000





Name: **$[(C_{12}NHC)_2\text{-}Ag]^+$ $[AgBr_2]^-$**

Qty of imaginary frequencies: 0

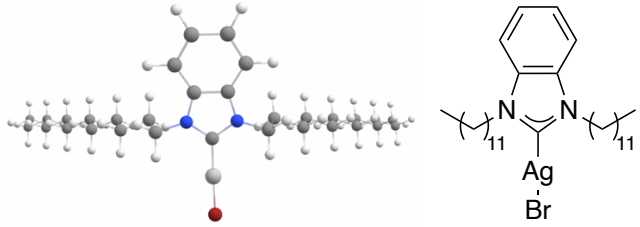
Final single point energy (Eh): -8087.09139255

Ag	17.558298000	8.387231000	13.188179000
N	17.389794000	6.767766000	15.832687000
N	17.387159000	5.444381000	14.109580000
C	17.392537000	6.750798000	14.474992000
C	17.369697000	5.475837000	16.338430000

C	17.378854000	4.621047000	15.225933000
C	17.382920000	4.984965000	12.723301000
H	17.638737000	5.857779000	12.113429000
H	18.199793000	4.264390000	12.596692000
C	17.318679000	7.986402000	16.638018000
H	17.720251000	8.801509000	16.024659000
H	17.997906000	7.872560000	17.490950000
C	15.892428000	8.291308000	17.101341000
H	15.569547000	7.550067000	17.845529000
H	15.917740000	9.261867000	17.614515000
C	14.884853000	8.321003000	15.955482000
H	14.837108000	7.323714000	15.496086000
H	15.245202000	8.992936000	15.161543000
C	13.477063000	8.731805000	16.382230000
H	13.209374000	8.213347000	17.314685000
H	13.452847000	9.807125000	16.610762000
C	11.021986000	8.850911000	15.651572000
H	10.783161000	8.566783000	16.687068000
H	10.966330000	9.949081000	15.616026000
C	13.583830000	4.720126000	11.858810000
H	13.732856000	4.692893000	10.768562000
H	13.474460000	3.671389000	12.173455000
C	12.439769000	8.396360000	15.313145000
H	12.441208000	7.307456000	15.155589000
H	12.744443000	8.838558000	14.353137000
C	14.834818000	5.303796000	12.513863000
H	15.041531000	6.306426000	12.110560000
H	14.664125000	5.438631000	13.591219000
C	16.042707000	4.391088000	12.295214000
H	16.131700000	4.148439000	11.227089000
H	15.866510000	3.437790000	12.811274000
C	11.095510000	4.804386000	11.454015000
H	11.275049000	4.822556000	10.368392000
H	11.057607000	3.741231000	11.734545000
C	12.280511000	5.457291000	12.164755000
H	12.364645000	6.512332000	11.863371000
H	12.104544000	5.462103000	13.250299000
C	8.561287000	8.761846000	14.964315000
H	8.308910000	8.640160000	16.028152000
H	8.524078000	9.843205000	14.763934000
C	9.735468000	5.436021000	11.743915000
H	9.739759000	6.491673000	11.432644000
H	9.551704000	5.440689000	12.828070000
C	6.106150000	4.500966000	10.580667000
H	6.309409000	4.481314000	9.499503000
H	6.128942000	3.452744000	10.913615000
C	8.602615000	4.695049000	11.034126000
H	8.799935000	4.688814000	9.951611000
H	8.612461000	3.641265000	11.349558000
C	7.513619000	8.049154000	14.113003000
H	7.532339000	6.973871000	14.344171000
H	7.788230000	8.132817000	13.050653000
C	6.097820000	8.582942000	14.315642000
H	5.828429000	8.512540000	15.380015000
H	6.070506000	9.654429000	14.065616000
C	7.215037000	5.278656000	11.287504000
H	7.193295000	6.327668000	10.955329000
H	7.016046000	5.300395000	12.368678000
C	9.976596000	8.247819000	14.715775000
H	9.991312000	7.153296000	14.826621000
H	10.258169000	8.446345000	13.670711000
C	17.368231000	4.980420000	17.637211000
H	17.365665000	5.638928000	18.499571000
C	17.402797000	3.238777000	15.373273000
H	17.434949000	2.572544000	14.517798000
C	17.380716000	3.597910000	17.783723000
H	17.382311000	3.170628000	18.781404000
C	17.401123000	2.743357000	16.672449000
H	17.422167000	1.669686000	16.829831000
C	3.613229000	4.284267000	10.111066000
H	2.623967000	4.713916000	10.299063000
H	3.596448000	3.242715000	10.451629000
H	3.773489000	4.276868000	9.027185000
C	4.710539000	5.073827000	10.820424000
H	4.687334000	6.120182000	10.484243000
H	4.510484000	5.098447000	11.900298000

C	5.056403000	7.842336000	13.479885000
H	5.336427000	7.902614000	12.419137000
H	5.081303000	6.774719000	13.738125000
C	3.641732000	8.381957000	13.670060000
H	3.314894000	8.271612000	14.710264000
H	2.922559000	7.855385000	13.033563000
H	3.591299000	9.448207000	13.420508000
N	18.276764000	10.041628000	10.663792000
N	17.353432000	11.298656000	12.176499000
C	17.703490000	10.018799000	11.894574000
C	18.283375000	11.330615000	10.150689000
C	17.695664000	12.143879000	11.131459000
C	16.698649000	11.711241000	13.415497000
H	16.804897000	10.870999000	14.109512000
H	17.268174000	12.544053000	13.844889000
C	18.733483000	8.849705000	9.950145000
H	18.940047000	8.083767000	10.706816000
H	19.692115000	9.082509000	9.471747000
C	17.707296000	8.357390000	8.927720000
H	17.640264000	9.061960000	8.087148000
H	18.086797000	7.412755000	8.515669000
C	16.317964000	8.155615000	9.525322000
H	15.927290000	9.126221000	9.861799000
H	16.391167000	7.537851000	10.433343000
C	15.314039000	7.532342000	8.557909000
H	15.391581000	8.025336000	7.577695000
H	15.562044000	6.474181000	8.390386000
C	12.836827000	6.983463000	8.183976000
H	13.009348000	7.259012000	7.133147000
H	12.959849000	5.891597000	8.237395000
C	12.897937000	11.353933000	12.591909000
H	12.575512000	11.334191000	13.644013000
H	12.756011000	12.391397000	12.253674000
C	13.880280000	7.663120000	9.066929000
H	13.636833000	8.732606000	9.152208000
H	13.813829000	7.258108000	10.087489000
C	14.385603000	11.012232000	12.523099000
H	14.572282000	10.027338000	12.977120000
H	14.698687000	10.925793000	11.473066000
C	15.229160000	12.080881000	13.220375000
H	14.819005000	12.281607000	14.219909000
H	15.145769000	13.022229000	12.661083000
C	10.518186000	10.855568000	11.910034000
H	10.224247000	10.779293000	12.967939000
H	10.420992000	11.919370000	11.646616000
C	11.983744000	10.445468000	11.771138000
H	12.109582000	9.398953000	12.087881000
H	12.279772000	10.483360000	10.712626000
C	10.338983000	6.621050000	7.777648000
H	10.550247000	6.715084000	6.702132000
H	10.395442000	5.546162000	8.006449000
C	9.541396000	10.046611000	11.059379000
H	9.611235000	8.980514000	11.324541000
H	9.829362000	10.114099000	10.000003000
C	5.656439000	10.271877000	10.570173000
H	5.385127000	10.232411000	11.635790000
H	5.619621000	11.333998000	10.285965000
C	8.100409000	10.525374000	11.229209000
H	7.822184000	10.458272000	12.291672000
H	8.044282000	11.592589000	10.968131000
C	8.927680000	7.130207000	8.059473000
H	8.866367000	8.193262000	7.782866000
H	8.731221000	7.090266000	9.141429000
C	7.841908000	6.352256000	7.319959000
H	8.045500000	6.375535000	6.239051000
H	7.887123000	5.292992000	7.615215000
C	7.082213000	9.752392000	10.394644000
H	7.120151000	8.686504000	10.666898000
H	7.362995000	9.800435000	9.332432000
C	11.409613000	7.364635000	8.571703000
H	11.281375000	8.447951000	8.430373000
H	11.259411000	7.181798000	9.645778000
C	18.759558000	11.859474000	8.956677000
H	19.220758000	11.234898000	8.198669000
C	17.575140000	13.518053000	10.958323000
H	17.142889000	14.154733000	11.722809000

C	18.629356000	13.232280000	8.779915000
H	18.991153000	13.685220000	7.862351000
C	18.050479000	14.046523000	9.763550000
H	17.977590000	15.115586000	9.591030000
C	3.202403000	10.036682000	9.938753000
H	2.477393000	9.465171000	9.350271000
H	3.137560000	11.084586000	9.624361000
H	2.895069000	9.985250000	10.989154000
C	4.619368000	9.497888000	9.758945000
H	4.650141000	8.438875000	10.052380000
H	4.895708000	9.526253000	8.696096000
C	6.437542000	6.890005000	7.583937000
H	6.247253000	6.883267000	8.665969000
H	6.391153000	7.943958000	7.276612000
C	5.348347000	6.098454000	6.865560000
H	5.480988000	6.142759000	5.778578000
H	4.350670000	6.485736000	7.098533000
H	5.373915000	5.042328000	7.157837000
Ag	20.335433000	8.635550000	13.836123000
Br	20.706961000	6.635487000	12.411148000
Br	19.762668000	10.611670000	15.226096000



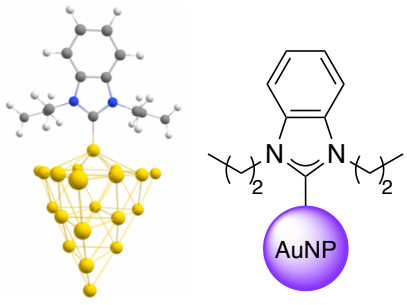
Name: **C_{12}NHC-AgBr**

Qty of imaginary frequencies: 0

Final single point energy (Eh): -4043.53292866

C	-0.996583000	-5.569880000	-3.953787000
N	-0.528690000	-5.224099000	-5.180990000
N	-2.340675000	-5.710273000	-4.088289000
C	0.870818000	-4.901098000	-5.451391000
H	1.115548000	-5.255875000	-6.460507000
H	1.474254000	-5.474855000	-4.738290000
C	1.153811000	-3.408446000	-5.306726000
H	0.517825000	-2.843173000	-6.001914000
H	0.869954000	-3.101230000	-4.290984000
C	2.624918000	-3.085009000	-5.556424000
H	2.910867000	-3.416355000	-6.565848000
H	3.245651000	-3.659209000	-4.853787000
C	2.934900000	-1.596725000	-5.404968000
H	2.640147000	-1.267661000	-4.398320000
H	2.317189000	-1.021667000	-6.110214000
C	4.408560000	-1.266290000	-5.634405000
H	4.706967000	-1.604486000	-6.637694000
H	5.023009000	-1.836920000	-4.923248000
C	4.718048000	0.222829000	-5.489937000
H	4.414477000	0.561109000	-4.488559000
H	4.105847000	0.793193000	-6.203924000
C	6.192865000	0.555265000	-5.710063000
H	6.498618000	0.211908000	-6.709349000
H	6.803925000	-0.011227000	-4.992394000
C	6.501004000	2.045311000	-5.571603000
H	6.191855000	2.388986000	-4.573639000
H	5.891816000	2.611433000	-6.291485000
C	7.976552000	2.378560000	-5.786039000
H	8.286761000	2.032303000	-6.782936000
H	8.585075000	1.814474000	-5.064194000
C	8.283772000	3.868938000	-5.650789000
H	7.972151000	4.216320000	-4.654687000
H	7.676699000	4.433665000	-6.373722000
C	9.759734000	4.204152000	-5.861842000
H	10.070807000	3.857016000	-6.856887000
H	10.365013000	3.640528000	-5.138546000
C	10.052866000	5.696696000	-5.724346000

H	9.779945000	6.060142000	-4.727128000
H	11.114263000	5.914675000	-5.880623000
H	9.480498000	6.278155000	-6.456082000
C	-3.236542000	-6.010112000	-2.972462000
H	-4.067230000	-6.616164000	-3.354880000
H	-2.670202000	-6.625731000	-2.263856000
C	-3.745536000	-4.745767000	-2.285833000
H	-2.877424000	-4.169108000	-1.938354000
H	-4.278085000	-4.118379000	-3.013815000
C	-4.656419000	-5.074923000	-1.105124000
H	-4.114926000	-5.723964000	-0.402071000
H	-5.524221000	-5.652590000	-1.456758000
C	-5.141004000	-3.828289000	-0.366921000
H	-5.676747000	-3.171947000	-1.068144000
H	-4.270128000	-3.257856000	-0.013982000
C	-6.047716000	-4.153419000	0.819062000
H	-5.513428000	-4.821177000	1.510152000
H	-6.924425000	-4.715690000	0.465215000
C	-6.514113000	-2.911657000	1.576886000
H	-7.044140000	-2.239240000	0.886427000
H	-5.636266000	-2.353940000	1.934057000
C	-7.421830000	-3.238107000	2.761969000
H	-6.894415000	-3.919445000	3.445369000
H	-8.304878000	-3.787586000	2.403922000
C	-7.874786000	-1.999930000	3.533729000
H	-8.399098000	-1.315531000	2.850726000
H	-6.991183000	-1.453670000	3.894799000
C	-8.784316000	-2.328089000	4.717044000
H	-8.262072000	-3.018646000	5.395274000
H	-9.671474000	-2.868285000	4.355100000
C	-9.228241000	-1.092461000	5.497723000
H	-9.747967000	-0.399170000	4.819977000
H	-8.341350000	-0.553985000	5.862943000
C	-10.140818000	-1.419855000	6.679327000
H	-9.621893000	-2.114096000	7.354560000
H	-11.027738000	-1.955179000	6.313066000
C	-10.573836000	-0.177009000	7.453965000
H	-11.118285000	0.519429000	6.806107000
H	-11.227710000	-0.433006000	8.293858000
H	-9.705279000	0.356558000	7.856391000
Br	1.315003000	-5.811894000	-0.119420000
C	-2.740296000	-5.426239000	-5.387162000
C	-1.569162000	-5.112095000	-6.093505000
C	-3.985287000	-5.420635000	-6.005372000
H	-4.894886000	-5.658154000	-5.463502000
C	-4.016861000	-5.089281000	-7.355389000
H	-4.969843000	-5.070986000	-7.874338000
C	-1.601160000	-4.781350000	-7.443230000
H	-0.699449000	-4.533781000	-7.993810000
C	-2.846879000	-4.775762000	-8.061037000
H	-2.915006000	-4.520492000	-9.113654000
Ag	0.081347000	-5.710143000	-2.205735000

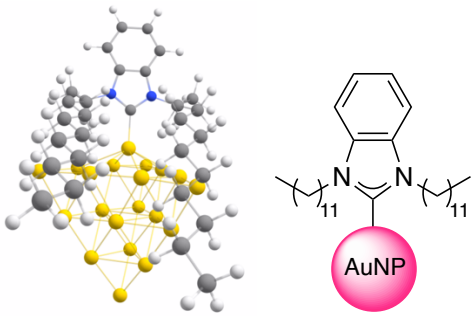


Name: **C_3NHC-AuNPs**

Qty of imaginary frequencies: 0

Final single point energy (Eh): -3332.31401534

Au	1.170987	-3.018682	-1.102078
Au	1.995139	-4.151279	1.244455
Au	2.703996	-4.877062	3.663888
Au	3.322971	-5.756698	6.155769
Au	-0.846987	-3.704999	0.578773
Au	-2.722514	-4.334232	2.377068
Au	-4.530180	-4.919653	4.322500
Au	-1.939800	-5.361084	5.043016
Au	0.647515	-5.654961	5.658387
Au	-0.010582	-4.826694	3.048183
Au	1.045234	-1.477211	1.134724
Au	-3.098876	-2.649476	4.759740
Au	2.332667	-3.237341	5.995428
Au	2.813119	-1.832118	3.310165
Au	-1.136905	-2.029919	2.812595
Au	-0.409991	-3.044417	5.568865
Au	0.704166	0.041239	3.265426
Au	1.259550	-0.844235	5.905127
Au	-1.563291	-0.490522	5.120090
Au	0.142216	1.600881	5.422005
N	5.770330	-2.154257	2.599858
N	5.534904	-0.988436	4.424988
C	4.851132	-1.689311	3.484388
C	7.042502	-1.724892	2.953471
C	8.288682	-1.917593	2.368596
C	6.891052	-0.974301	4.127372
C	9.378204	-1.330930	3.001888
H	8.411327	-2.492341	1.456662
C	7.980516	-0.387381	4.760591
C	9.226758	-0.579658	4.175731
H	10.368469	-1.454807	2.575549
H	7.869615	0.200752	5.665415
H	10.102511	-0.135064	4.637356
C	4.924268	-0.281760	5.549673
H	4.057444	-0.870646	5.880108
H	5.651840	-0.273024	6.370298
C	4.489386	1.133850	5.183066
H	3.742396	1.066878	4.380209
H	5.347144	1.692377	4.785689
C	3.894948	1.848470	6.392139
H	3.538638	2.846693	6.120666
H	3.037924	1.287065	6.788017
H	4.629516	1.958128	7.198313
C	5.463072	-2.929276	1.399251
H	4.596659	-3.566246	1.626725
H	6.316909	-3.589600	1.203773
C	5.164916	-2.045157	0.192142
H	5.990082	-1.336701	0.041015
H	4.264160	-1.454787	0.409931
C	4.950189	-2.889900	-1.059420
H	4.684166	-2.261270	-1.914504
H	5.851287	-3.456029	-1.322084
H	4.132484	-3.607068	-0.907578



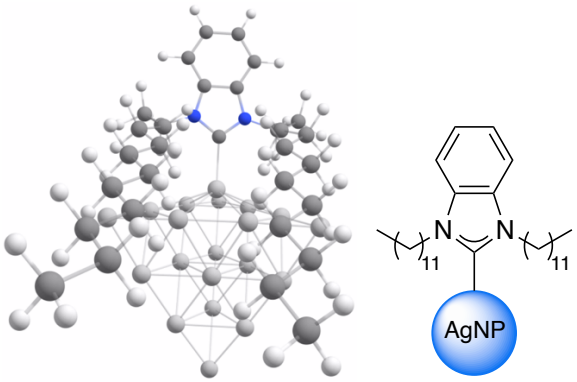
Name: **C_{12}NHC-AuNP**

Qty of imaginary frequencies: 0

Final single point energy (Eh): -4039.24882089

N	4.228815	-1.493203	14.790703
N	3.010761	-3.286919	14.574791
C	4.290150	-2.827162	14.531575
C	2.912996	-1.095861	14.984022
C	2.130043	-2.248679	14.844115
C	2.597667	-4.660360	14.292697
H	3.495711	-5.282362	14.393346
H	1.888137	-4.969732	15.070108
C	5.369614	-0.578759	14.792756
H	6.267508	-1.201566	14.901147
H	5.295039	0.055502	15.684784
C	5.467781	0.260858	13.517391
H	4.670104	1.015107	13.486409
H	6.417831	0.809642	13.584026
C	5.452300	-0.581472	12.244790
H	4.439640	-0.963558	12.052343
H	6.080399	-1.474451	12.402162
C	5.978422	0.149968	11.015111
H	5.367884	1.041698	10.808907
H	6.996128	0.511497	11.229564
C	6.662892	-0.079032	8.570470
H	6.118393	0.847196	8.332935
H	7.687516	0.225657	8.829881
C	2.656253	-4.827433	10.420539
H	2.873486	-5.907045	10.494305
H	1.603333	-4.746939	10.114333
C	6.021154	-0.750272	9.781404
H	5.001716	-1.077437	9.527868
H	6.580315	-1.667413	10.030693
C	2.874711	-4.212602	11.797925
H	3.934121	-4.355668	12.060497
H	2.719045	-3.125133	11.757108
C	2.002429	-4.828648	12.891821
H	1.909694	-5.910905	12.725862
H	0.985926	-4.416502	12.847612
C	3.765835	-5.097037	8.137768
H	4.097688	-6.099567	8.484200
H	2.805756	-5.266612	7.628747
C	3.573369	-4.211233	9.363555
H	4.562911	-4.031015	9.818568
H	3.196069	-3.223894	9.061783
C	7.357170	-0.299938	6.128995
H	6.827881	0.637756	5.903388
H	8.386654	-0.014045	6.389606
C	4.802428	-4.561083	7.157075
H	5.728071	-4.333044	7.707125
H	4.452737	-3.605959	6.738517
C	6.515834	-5.979926	3.933098
H	6.899009	-6.910987	4.376123
H	5.602761	-6.255396	3.384881
C	5.118670	-5.534342	6.023242
H	5.477765	-6.481073	6.455408
H	4.195390	-5.776137	5.476565
C	7.377606	-1.179703	4.880908
H	6.347301	-1.464252	4.620759
H	7.903131	-2.119196	5.105973
C	8.034397	-0.506260	3.677733
H	7.502905	0.428891	3.446716
H	9.062680	-0.215806	3.938717
C	6.162891	-4.996998	5.047866
H	7.075023	-4.735519	5.603935
H	5.798982	-4.058665	4.604447
C	6.701679	-0.973219	7.333262
H	5.677570	-1.276969	7.070435
H	7.240916	-1.901561	7.573233
C	2.345530	0.137648	15.282660
H	2.947975	1.032170	15.399075
C	0.748515	-2.213785	14.995130
H	0.138878	-3.105139	14.892637
C	0.963620	0.174129	15.430482
H	0.480537	1.117737	15.662975
C	0.179839	-0.979663	15.289115
H	-0.895868	-0.908295	15.413844
C	7.908529	-6.417340	1.846864
H	8.643138	-5.995753	1.153167
H	7.023090	-6.699375	1.265827

H	8.333979	-7.335231	2.268036
C	7.545572	-5.425675	2.950071
H	8.451713	-5.137777	3.501221
H	7.154958	-4.501624	2.502206
C	8.062418	-1.391782	2.433069
H	8.601383	-2.320462	2.665100
H	7.035520	-1.690821	2.179662
C	8.709942	-0.707691	1.231259
H	8.169080	0.206270	0.960400
H	8.721477	-1.362082	0.353594
H	9.745673	-0.425748	1.451994
Au	9.682000	-0.840764	13.402967
Au	10.836117	-3.308624	13.567971
Au	11.780321	-5.800194	13.760359
Au	12.589305	-8.387702	13.968813
Au	8.158718	-2.857113	12.404892
Au	6.754834	-4.842359	11.408348
Au	5.487118	-7.011030	10.341723
Au	7.885196	-7.607608	11.442666
Au	10.239820	-8.051153	12.635937
Au	9.313502	-5.389450	12.418287
Au	8.516587	-2.516551	15.209990
Au	5.563250	-6.804091	13.066672
Au	10.490657	-7.750500	15.578125
Au	9.617682	-5.062399	15.432771
Au	5.991769	-3.915693	14.066730
Au	8.012490	-7.411696	14.262703
Au	7.297342	-4.256002	16.751666
Au	8.368907	-7.017207	17.031520
Au	5.801397	-6.446505	15.658334
Au	6.146589	-6.142464	18.333709



Name: **C_{12}NHC-AgNP**

Qty of imaginary frequencies: 0

Final single point energy (Eh): -4264.13265165

N	4.030490000	-1.590028000	14.657001000
N	2.954310000	-3.470055000	14.628178000
C	4.201966000	-2.933472000	14.503392000
C	2.694852000	-1.269471000	14.861867000
C	1.999252000	-2.484380000	14.839197000
C	2.631750000	-4.883634000	14.458182000
H	3.571498000	-5.434408000	14.600204000
H	1.947052000	-5.183158000	15.261578000
C	5.101292000	-0.601768000	14.583653000
H	6.040726000	-1.156711000	14.713785000
H	5.000832000	0.080823000	15.437499000
C	5.134856000	0.167308000	13.263307000
H	4.281640000	0.854787000	13.191236000
H	6.037768000	0.793843000	13.298005000
C	5.191120000	-0.737901000	12.033260000
H	4.194040000	-1.138897000	11.804527000

H	5.817345000	-1.616543000	12.262792000
C	5.778280000	-0.039210000	10.812459000
H	5.191838000	0.858844000	10.567237000
H	6.789244000	0.317217000	11.075829000
C	6.661139000	-0.271665000	8.448852000
H	6.183746000	0.688265000	8.201037000
H	7.671408000	-0.025088000	8.810472000
C	2.709449000	-5.240849000	10.590811000
H	2.954880000	-6.314753000	10.679737000
H	1.661834000	-5.190841000	10.261095000
C	5.887253000	-0.939094000	9.583262000
H	4.883132000	-1.225437000	9.238044000
H	6.391519000	-1.879153000	9.867138000
C	2.888499000	-4.588842000	11.955379000
H	3.953088000	-4.672276000	12.229729000
H	2.687209000	-3.510920000	11.880762000
C	2.050790000	-5.198440000	13.076010000
H	2.038197000	-6.293465000	12.981067000
H	1.008031000	-4.862768000	13.003081000
C	3.776498000	-5.384062000	8.257220000
H	4.126926000	-6.402662000	8.492608000
H	2.796934000	-5.497429000	7.770332000
C	3.631841000	-4.601123000	9.556822000
H	4.636164000	-4.494663000	10.007421000
H	3.293338000	-3.576897000	9.342916000
C	7.596615000	-0.413906000	6.096049000
H	7.150994000	0.570570000	5.889420000
H	8.607529000	-0.214820000	6.481149000
C	4.764422000	-4.720632000	7.301206000
H	5.721249000	-4.575756000	7.826123000
H	4.402822000	-3.712684000	7.049099000
C	6.299414000	-5.569622000	3.803779000
H	6.684636000	-6.569820000	4.050856000
H	5.362356000	-5.730443000	3.250442000
C	5.013827000	-5.505085000	6.016062000
H	5.392136000	-6.506613000	6.268439000
H	4.062600000	-5.659052000	5.485638000
C	7.702397000	-1.197493000	4.789145000
H	6.693508000	-1.384177000	4.392591000
H	8.138926000	-2.187193000	4.987146000
C	8.536639000	-0.473546000	3.732950000
H	8.104235000	0.520920000	3.547100000
H	9.547781000	-0.296379000	4.128137000
C	6.006479000	-4.803618000	5.091483000
H	6.947404000	-4.634943000	5.636256000
H	5.621618000	-3.804287000	4.840097000
C	6.778810000	-1.115028000	7.180589000
H	5.774370000	-1.342967000	6.794233000
H	7.240202000	-2.083451000	7.424084000
C	2.041886000	-0.061629000	15.081208000
H	2.576826000	0.881837000	15.108476000
C	0.622947000	-2.539006000	15.028675000
H	0.080521000	-3.478532000	15.014371000
C	0.664907000	-0.114924000	15.269449000
H	0.117455000	0.806140000	15.442425000
C	-0.031974000	-1.330977000	15.242444000
H	-1.106716000	-1.329776000	15.393906000
C	7.589763000	-5.596924000	1.605051000
H	8.308393000	-5.055359000	0.980957000
H	6.674322000	-5.734076000	1.018306000
H	8.004806000	-6.590667000	1.808188000
C	7.300978000	-4.848117000	2.903543000
H	8.237210000	-4.696312000	3.458717000
H	6.919988000	-3.843587000	2.674874000
C	8.640377000	-1.230257000	2.409677000
H	9.070937000	-2.223974000	2.593631000
H	7.630596000	-1.404492000	2.012732000
C	9.479045000	-0.489671000	1.370178000
H	9.050503000	0.494443000	1.148574000
H	9.539565000	-1.047436000	0.430045000
H	10.501450000	-0.331165000	1.731587000
Ag	5.236941000	-7.729049000	11.199540000
Ag	7.797780000	-7.895426000	12.167839000
Ag	10.326458000	-7.946846000	13.209289000
Ag	10.816702000	-7.000893000	15.888395000
Ag	12.847100000	-7.920533000	14.292448000

```
Ag      11.753586000     -5.496644000     13.620818000
Ag       9.675473000     -4.513889000     15.241130000
Ag       9.149695000     -5.477881000     12.535078000
Ag       8.744936000     -6.041397000     17.394407000
Ag       8.216033000     -7.032128000     14.823872000
Ag      10.586985000     -3.113397000     12.966707000
Ag       7.877483000     -3.077232000     11.975383000
Ag       8.414960000     -2.149078000     14.562532000
Ag       9.282032000     -0.767643000     12.355647000
Ag       7.490096000     -3.542204000     16.663467000
Ag       6.136247000     -3.995395000     14.140153000
Ag       6.602923000     -5.029632000     18.777763000
Ag       6.533600000     -5.354542000     11.597011000
Ag       6.092982000     -5.971106000     16.265997000
Ag       5.659303000     -6.885801000     13.775655000
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1.5. Comparison of calculation time for r^{2}scan-3c versus B3LYP/DEF2-TZVPD

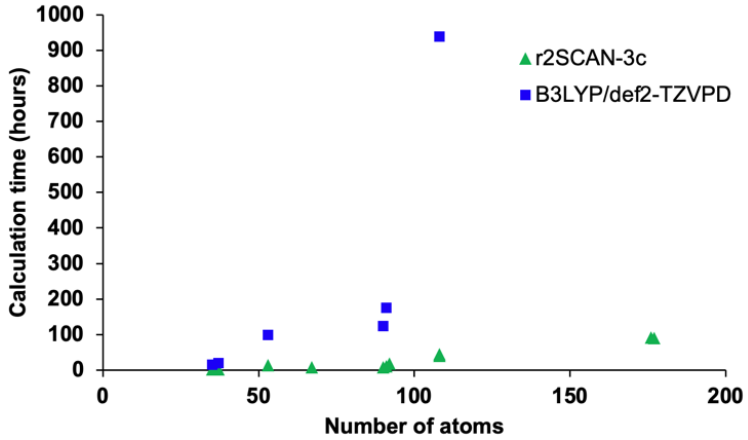


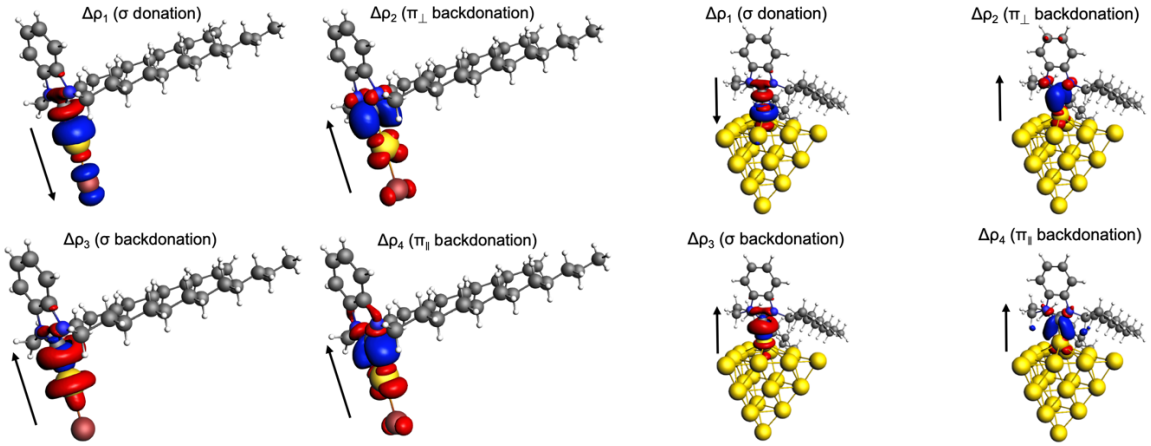
Figure S1. Computational time required for a geometry optimization and frequency calculation (using 16-cores) as a function of the total number of atoms using B3LYP/def2-TZVPD (blue squares) and r^{2}SCAN-3c (green triangles).

1.6. EDA-NOCV calculation:

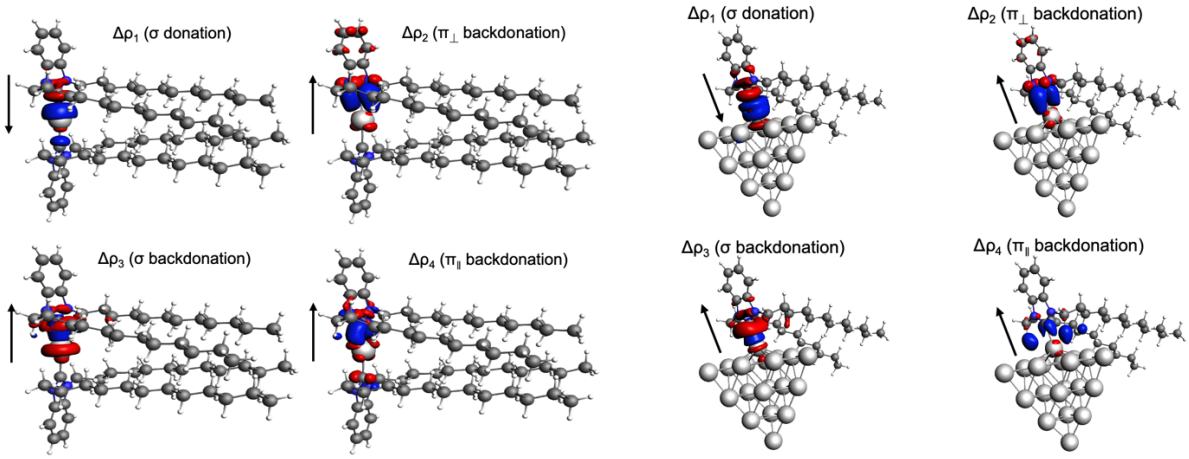
Table S1. Bond energy decomposition analysis of each complex and nanoparticle (kcal/mol).

Energies (kcal/mol)	C_{12}NHC-AuBr	$[(C_{12}NHC)_2\text{-}Ag]^+ [AgBr_2]^-$	C_3NHC-AuBr	C_{12}NHC-AuNP	C_{12}NHC-AgNP	C_3NHC-AuNP
ΔE_{int}	-85.43	-79.81	-84.33	-69.89	-49.49	-67.29
ΔE_{Pauli}	210.36	143.65	198.46	258.86	136.58	248.01
ΔV_{elstat}	-219.45	-155.02	-209.95	-218.27	-124.53	-214.23
ΔE_{oi}	-74.03	-53.99	-71.09	-99.16	-51.33	-93.22
ΔE_{disp}	-2.31	-14.45	-1.75	-11.32	-10.21	-7.85
Total Bonding Energy	-85.06	-78.46	-83.99	-68.94	-48.84	-66.70

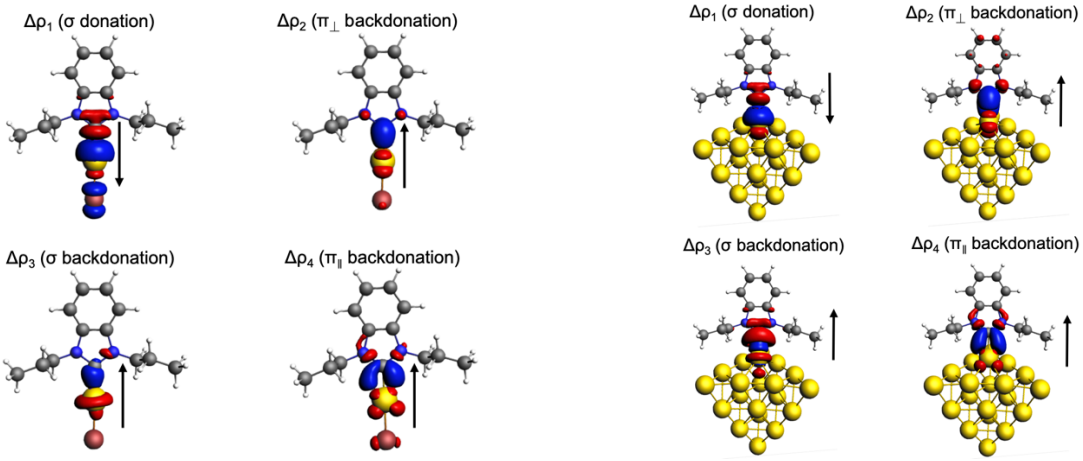
C_{12}NHC-Au :



C_{12}NHC-Ag :



C_3NHC-Au :



Red surfaces = loss of electron density/depletion of electron density); blue surfaces = gain of electron density/accumulation of electron density. Arrow indicates the direction of electron flow after bonding.

1.7. Raman Assignment

Table S2. Experimental and DFT Raman bands of **C_{12}NHC-AuBr** in the 100-1700 cm^{-1} region. Obtained with r^2SCAN-3c TightOpt TightSCF

Mode	Experimental Frequency (ν_{exp}, cm^{-1})	DFT Harmonic Frequency (cm^{-1})	(DFT Frequency)*0.98 (ν_{DFT}, cm^{-1})	Deviation ($\nu_{exp} - \nu_{DFT}$, cm^{-1})
ν_1	196	197.1	193.2	2.8
ν_2	237	243.1	238.2	-1.2
ν_3	555	555.4	544.3	10.7
ν_4	645	646.2	633.2	11.8
ν_5	752	744.9	730.0	22
ν_6	894	901.8	883.7	10.3
ν_7	1018	1035.6	1014.9	3.1
ν_8	1182	1205.6	1181.5	0.5
ν_9	1299	1325.3	1298.8	0.2
ν_{10}	1376	1400.2	1372.2	3.8
ν_{11}	1420	1432.6	1403.9	16.1
ν_{12}	1445	1476.6	1447.0	-2
ν_{13}	1614	1644.7	1611.8	2.2
			RMSD[1] =	9.4

[1]RMSD = Root Mean Square Deviation between experimental and DFT-calculated vibrational modes

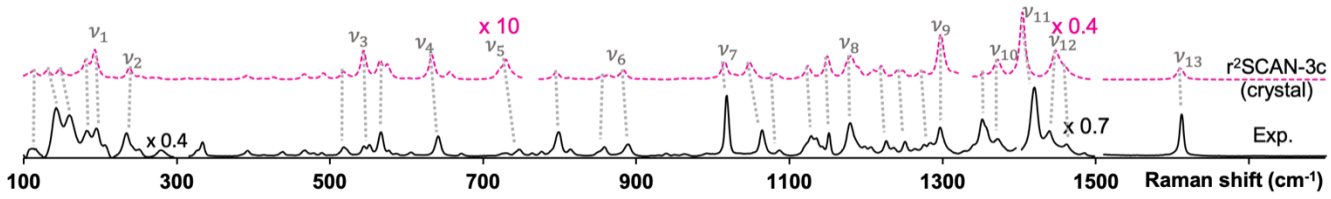
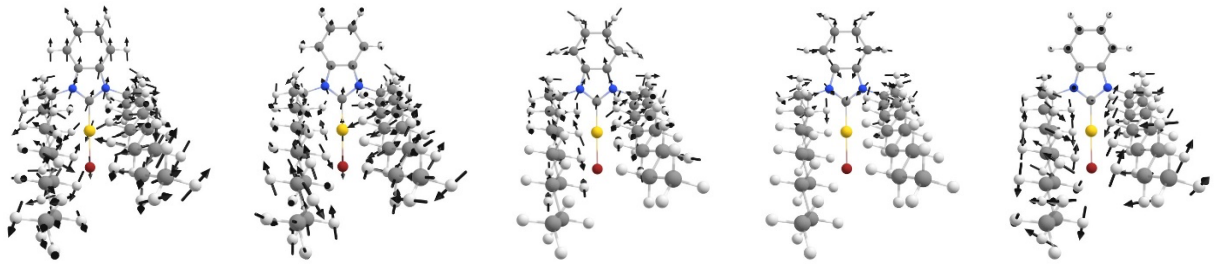


Figure S2. Experimental and predicted (r^2SCAN-3c TightOpt TightSCF) Raman spectrum of **C_3NHC-AgBr** in the 100-1700 cm^{-1} region



ν_1 **ν_2** **ν_3** **ν_4** **ν_5**

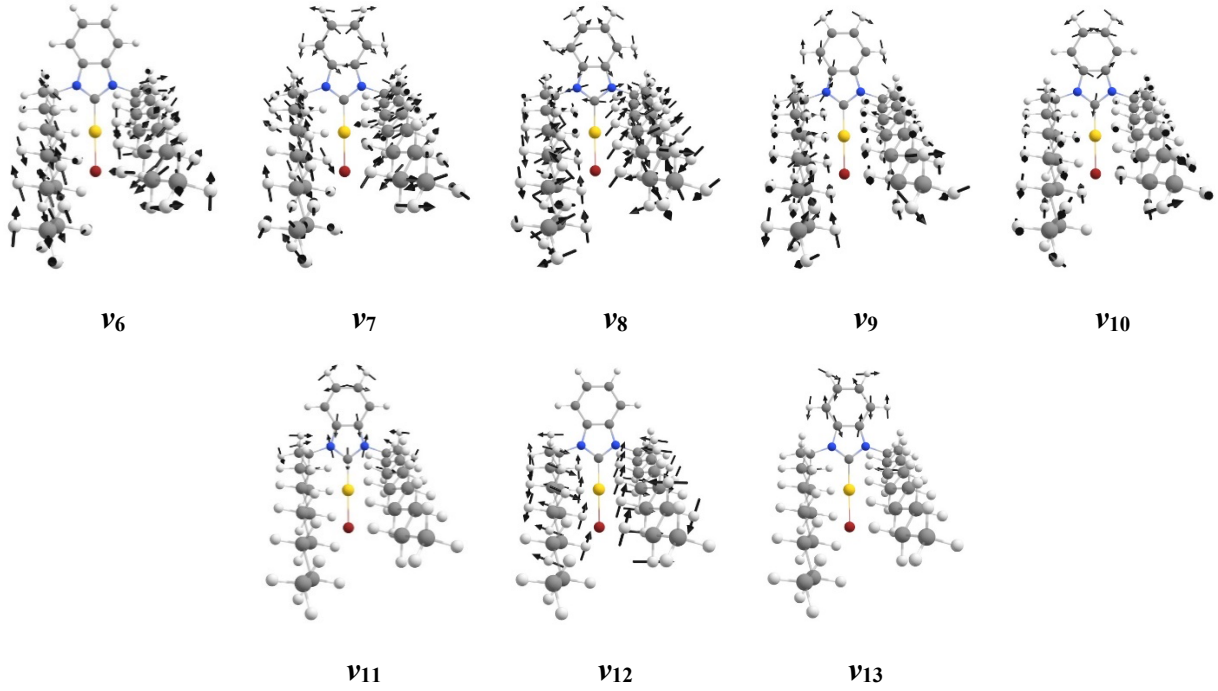


Table S3. Experimental and DFT Raman bands of **$[(C_{12}NHC)_2\text{-}Ag]^+$ $[AgBr_2]^-$** in the 100-1700 cm^{-1} region. Obtained with r^2SCAN-3c TightOpt TightSCF

Mode	Experimental Frequency (ν_{exp}, cm^{-1})	DFT Harmonic Frequency (cm^{-1})	(DFT Frequency)*0.98 (ν_{DFT}, cm^{-1})	Deviation ($\nu_{exp} - \nu_{DFT}$, cm^{-1})
ν_1	ND	142	140	0.0
ν_2	141.6	157	154	-12.3
ν_3	165.6	181	178	-11.9
ν_4	233.3	238	234	-0.3
ν_5	790.7	807	791	-0.4
ν_6	1018.1	1038	1017	1.3
ν_7	1131.6	1148	1126	6.1
ν_8	1155.7	1172	1148	7.4
ν_9	1300.5	1319	1293	7.4
ν_{10}	1370.3	1407	1378	-8.2
ν_{11}	1412.3	1431	1402	9.8
ν_{12}	1457.9	1485	1455	3.0
ν_{13}	1612.5	1641	1608	4.7
			RMSD[1] =	7.0

[1]RMSD = Root Mean Square Deviation between experimental and DFT-calculated vibrational modes

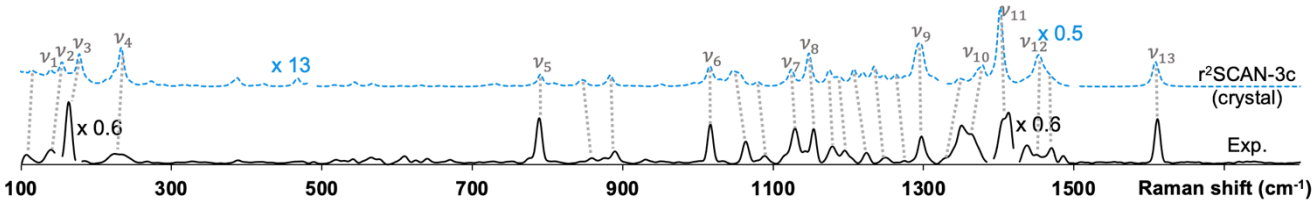


Figure S3. Experimental and predicted (r^2SCAN-3c TightOpt TightSCF) Raman spectrum of **$[(C_{12}NHC)_2\text{-}Ag]^+$ $[AgBr_2]^-$** in the 100-1700 cm^{-1} region

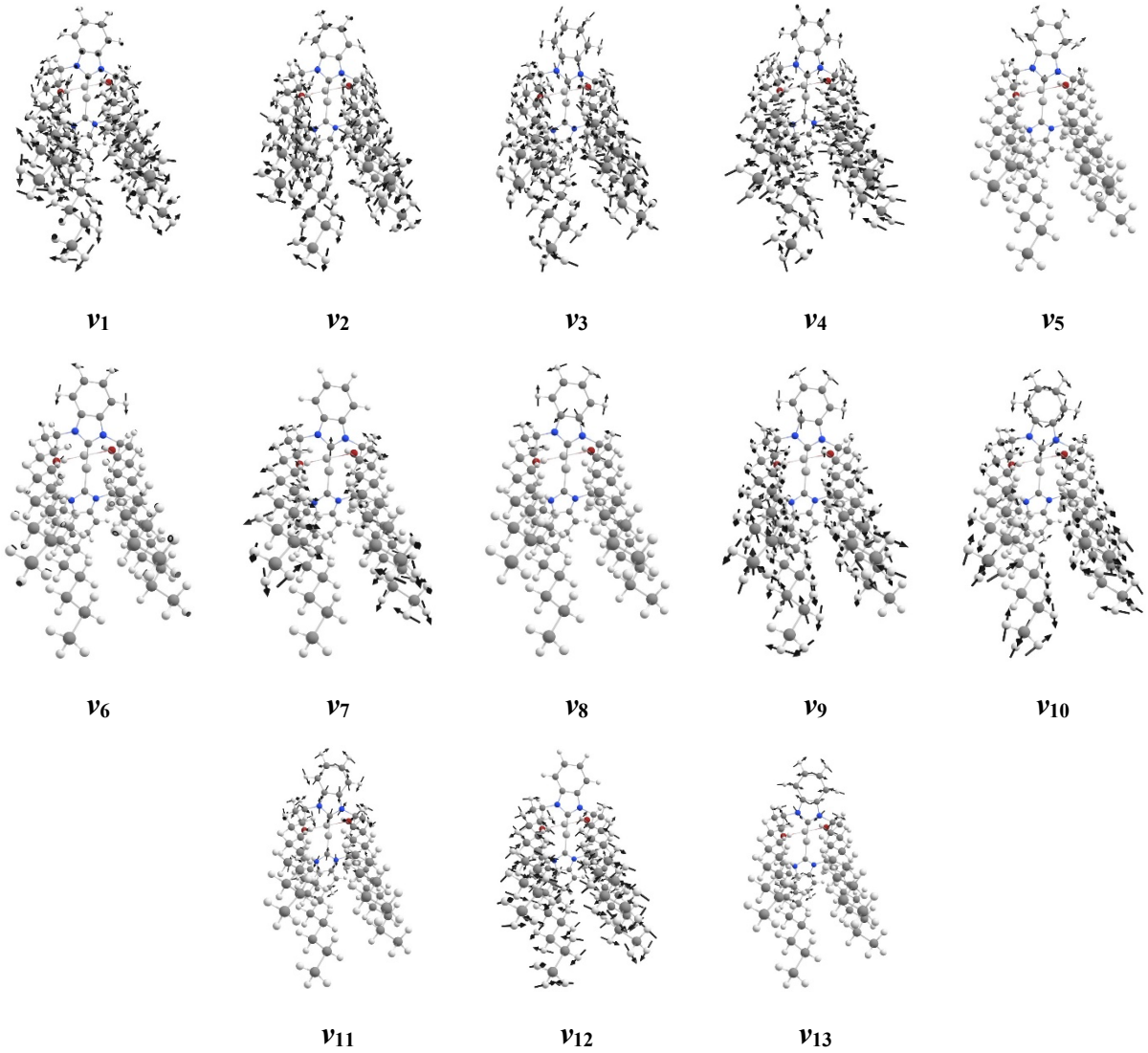


Table S4. Experimental and DFT Raman bands of **C_3NHC-AuBr** in the 100-1700 cm^{-1} region. Obtained with r^{2}SCAN-3c TightOpt TightSCF

Mode	Experimental Frequency (ν_{exp}, cm^{-1})	DFT Harmonic Frequency (cm^{-1})	(DFT Frequency)*0.98 (ν_{DFT}, cm^{-1})	Deviation ($\nu_{exp} - \nu_{DFT}$, cm^{-1})
ν_1	131	119.5	117.1	13.9
ν_2	177	179.2	175.6	1.4
ν_3	246	251.5	246.5	-0.5
ν_4	397	369.7	362.3	34.7
ν_5	553	580.4	568.8	-15.8
ν_6	589	619.6	607.2	-18.2
ν_7	682	685.5	671.8	10.2
ν_8	803	816.8	800.5	2.5
ν_9	889	898.7	880.8	8.2
ν_{10}	1017	1036.7	1016.0	1.0
ν_{11}	1133	1148.5	1125.6	7.4
ν_{12}	1157	1173.0	1149.6	7.4
ν_{13}	1180	1201.1	1177.1	2.9
ν_{14}	1235	1259.4	1234.2	0.8
ν_{15}	1363	1392.6	1364.7	-1.7
ν_{16}	1423	1435.0	1406.3	16.7
ν_{17}	1444	1476.0	1446.5	-2.5
ν_{18}	1612	1645.9	1613.0	-1.0
			RMSD[1] =	11.9

[1]RMSD = Root Mean Square Deviation between experimental and DFT-calculated vibrational modes

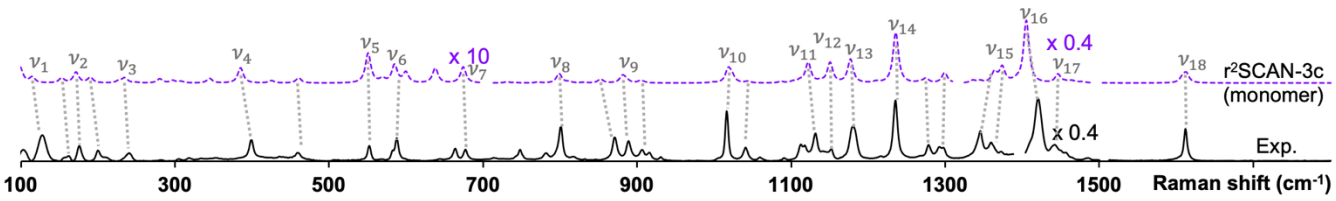
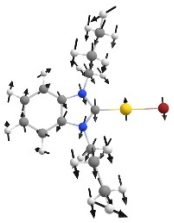
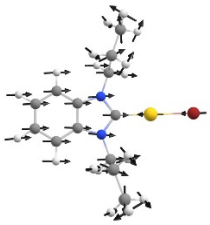


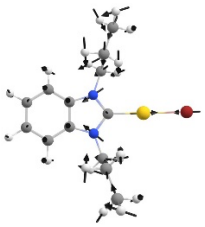
Figure S4. Experimental and predicted (r^{2}SCAN-3c TightOpt TightSCF) Raman spectrum of **C_3NHC-AuBr** in the 100-1700 cm^{-1} region



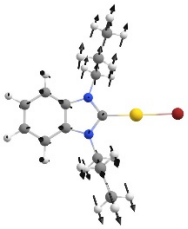
ν_1



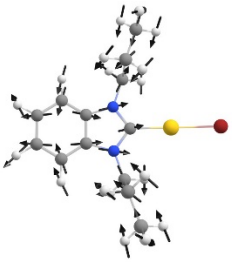
ν_2



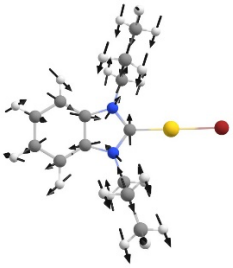
ν_3



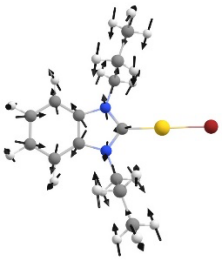
ν_4



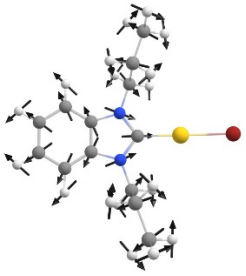
ν_5



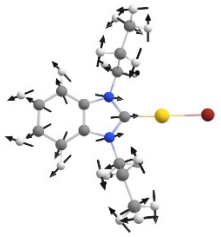
ν_6



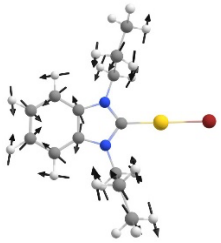
ν_7



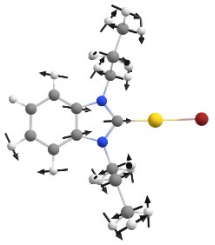
ν_8



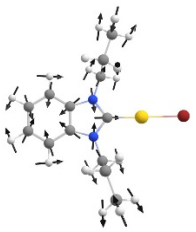
ν_9



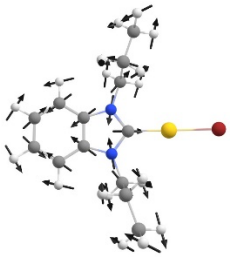
ν_{10}



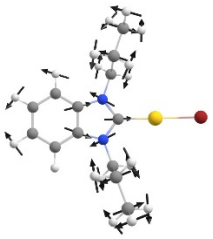
ν_{11}



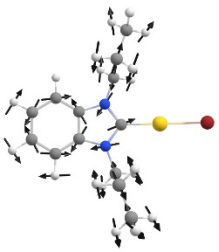
ν_{12}



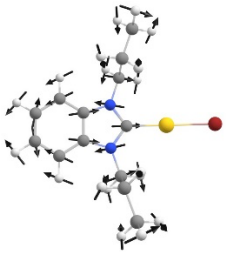
ν_{13}



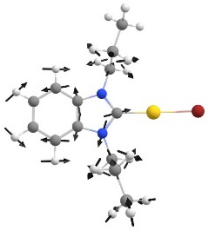
ν_{14}



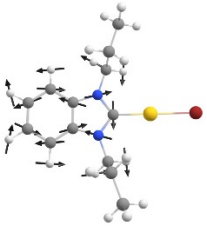
ν_{15}



ν_{16}



ν_{17}



ν_{18}

Table S5. Experimental and DFT Raman bands of **C_{12}NHC-AuNP** in the 100-1700 cm^{-1} region. Obtained with r^2SCAN-3c TightOpt TightSCF

Mode	Experimental Frequency (ν_{exp}, cm^{-1})	DFT Harmonic Frequency (cm^{-1})	(DFT Frequency)*0.98 (ν_{DFT}, cm^{-1})	Deviation ($\nu_{exp} - \nu_{DFT}$, cm^{-1})
ν_1	143	124.9	122.4	20.6
ν_2	156	145.9	143.0	13.0
ν_3	531	552.5	541.5	-10.5
ν_4	735	730.4	715.8	19.2
ν_5	796	805.8	789.6	6.4
ν_6	1019	1037.8	1017.0	2.0
ν_7	1138	1141.5	1118.7	19.3
ν_8	1160	1171.8	1148.4	11.6
ν_9	1216	1229.3	1204.7	11.3
ν_{10}	1304	1324.6	1298.1	5.9
ν_{11}	1424	1421.5	1393.1	30.9
ν_{12}	1473	1485.1	1455.4	17.6
ν_{13}	1614	1643.5	1610.6	3.4
			RMSD[1] =	15.4

[1]RMSD = Root Mean Square Deviation between experimental and DFT-calculated vibrational modes

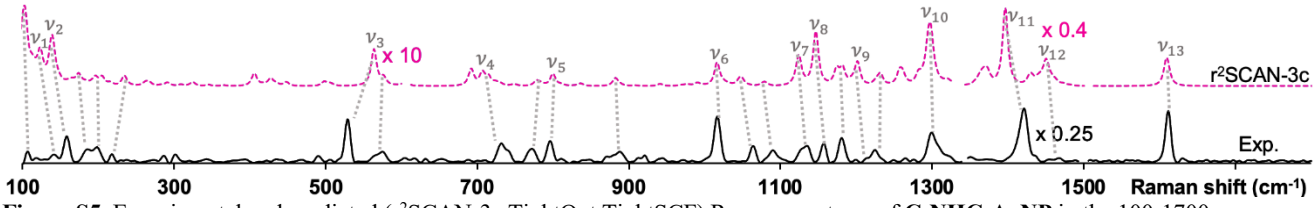
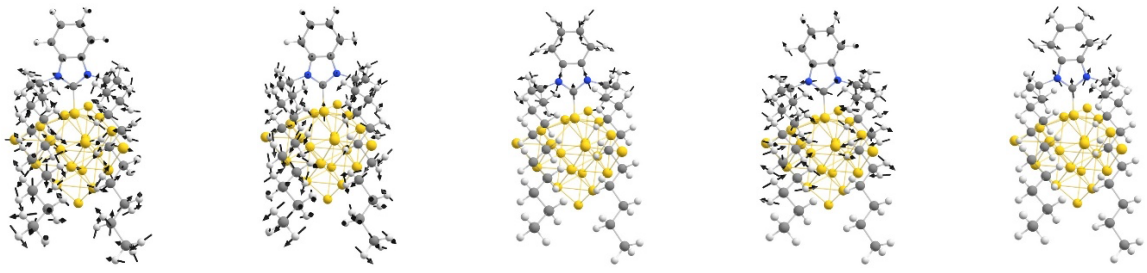


Figure S5. Experimental and predicted (r^2SCAN-3c TightOpt TightSCF) Raman spectrum of **C_3NHC-AgNP** in the 100-1700 cm^{-1} region



ν_1 **ν_2** **ν_3** **ν_4** **ν_5**

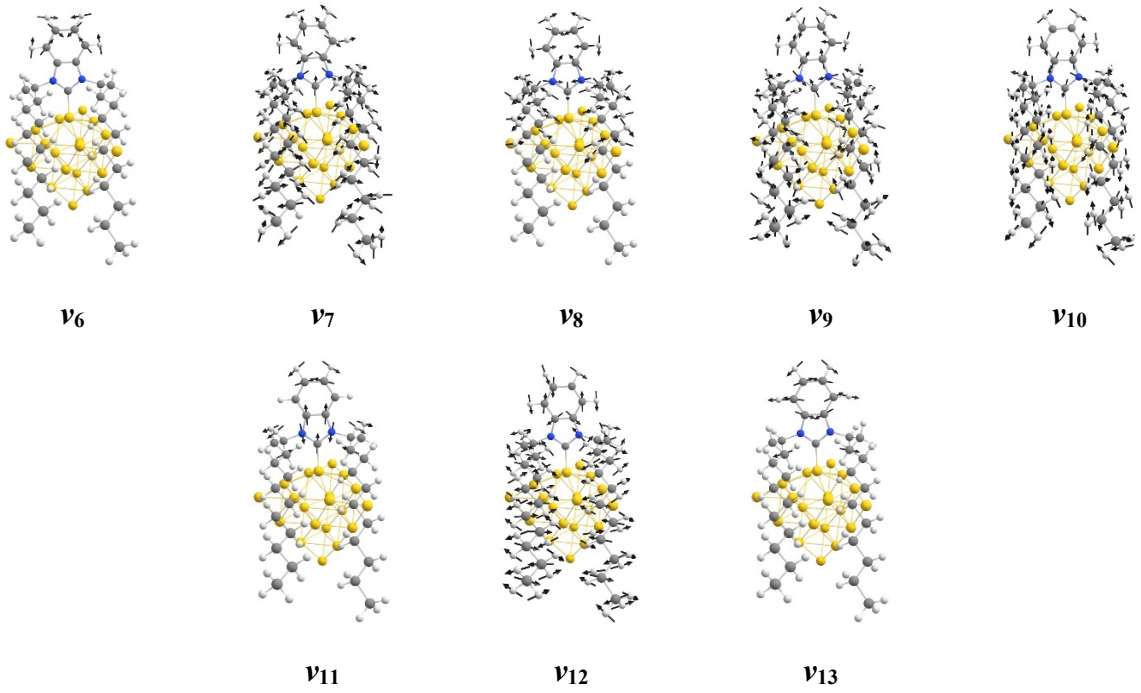


Table S6. Experimental and DFT Raman bands of **C_{12}NHC-AgNP** in the 100-1700 cm^{-1} region. Obtained with r^2SCAN-3c TightOpt TightSCF

Mode	Experimental Frequency (ν_{exp}, cm^{-1})	DFT Harmonic Frequency (cm^{-1})	(DFT Frequency)*0.98 (ν_{DFT}, cm^{-1})	Deviation ($\nu_{exp} - \nu_{DFT}$, cm^{-1})
ν_1	113.43	123	121	-7.4
ν_2	ND	142	139	0.0
ν_3	ND	163	160	0.0
ν_4	177.64	186	182	-4.2
ν_5	ND	730	715	0.0
ν_6	776.24	797	781	-4.4
ν_7	883.15	902	884	-0.7
ν_8	1015.28	1036	1016	-0.2
ν_9	1136.7	1170	1147	-10.1
ν_{10}	1301.24	1320	1293	7.8
ν_{11}	1352.27	1389	1361	-9.2
ν_{12}	1357.13	1415	1386	-29.1
ν_{13}	1425.18	1483	1453	-27.7
ν_{14}	1610.42	1643	1610	0.3
			RMSD[1] =	11.8

[1]RMSD = Root Mean Square Deviation between experimental and DFT-calculated vibrational modes

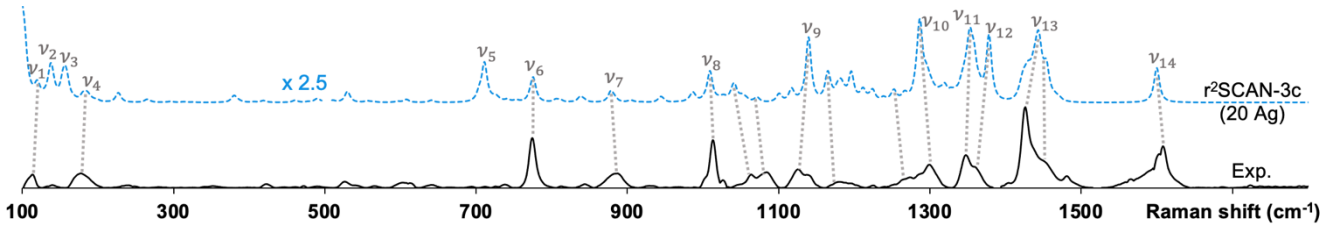
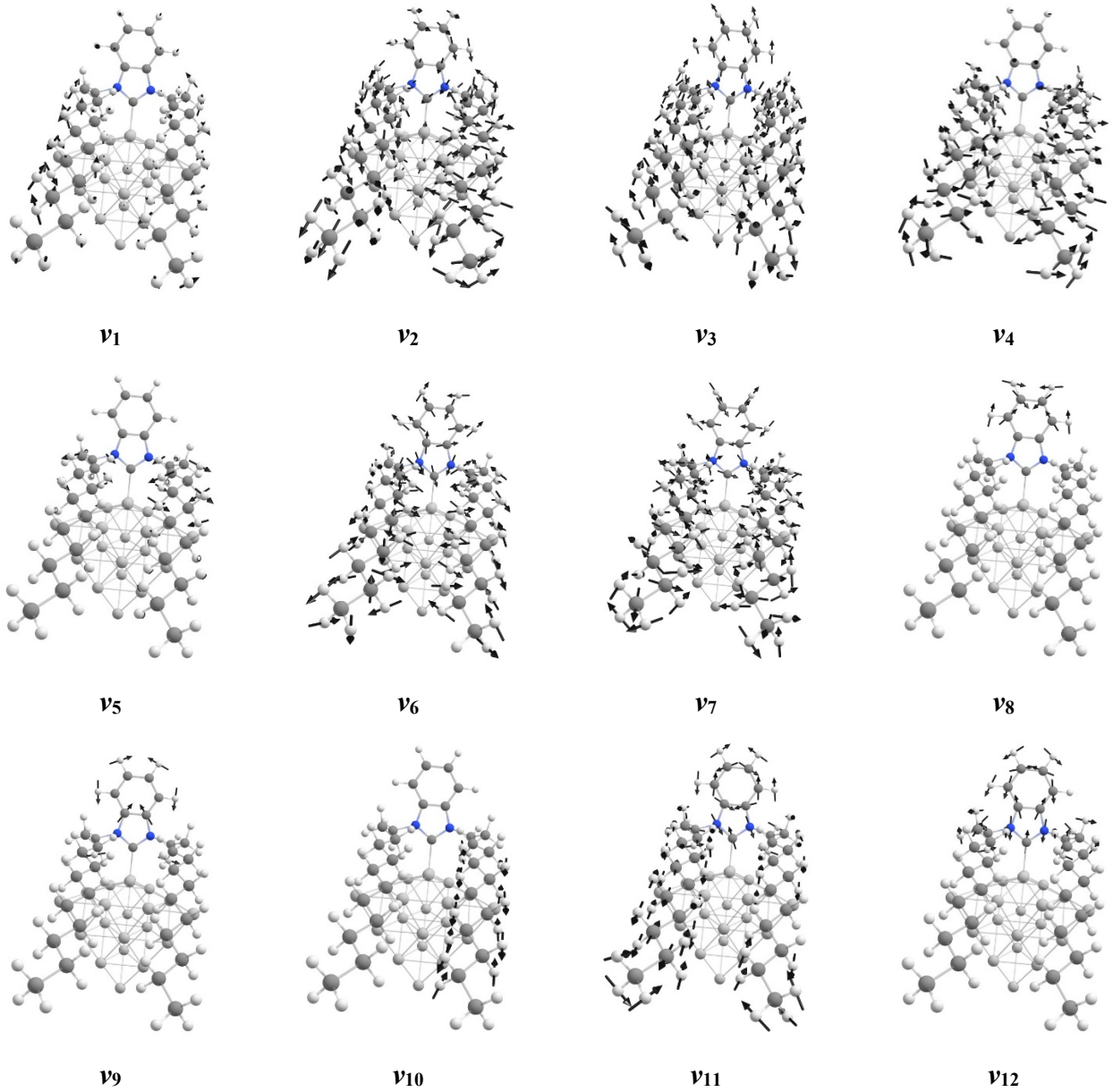
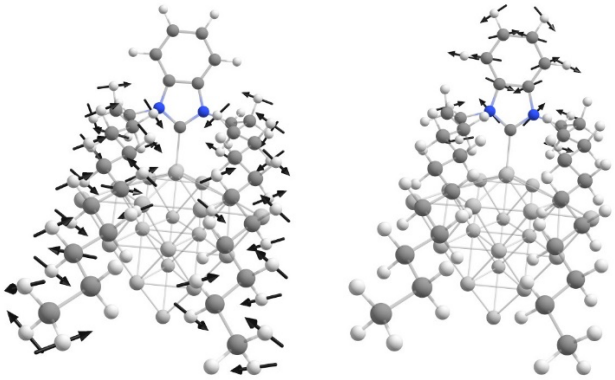


Figure S6. Experimental and predicted (r[2]SCAN-3c TightOpt TightSCF) Raman spectrum of **C_{12}NHC-AgNP** in the 100-1700 cm^{-1} region





ν_{13} ν_{14}

Table S7. Experimental and DFT Raman bands of **C_3NHC-AuNP** in the 100-1700 cm^{-1} region. Obtained with r^2SCAN-3c TightOpt TightSCF

Mode	Experimental Frequency (ν_{exp}, cm^{-1})	DFT Harmonic Frequency (cm^{-1})	(DFT Frequency)*0.98 (ν_{DFT}, cm^{-1})	Deviation ($\nu_{exp} - \nu_{DFT}$, cm^{-1})
ν_1	133	122.0	119.6	13.4
ν_2	182	141.6	138.8	43.2
ν_3	236	227.7	223.2	12.8
ν_4	346	346.2	339.2	6.8
ν_5	793	810.6	794.4	-1.4
ν_6	1018	1039.7	1018.9	-0.9
ν_7	1123	1142.4	1119.6	3.4
ν_8	1149	1173.7	1150.2	-1.2
ν_9	1177	1201.7	1177.7	-0.7
ν_{10}	1231	1253.9	1228.9	2.1
ν_{11}	1297	1316.1	1289.8	7.2
ν_{12}	1357	1391.8	1363.9	-6.9
ν_{13}	1399	1426.1	1397.5	1.5
ν_{14}	1614	1641.8	1609.0	4.7
			RMSD[1] =	13.1

[1]RMSD = Root Mean Square Deviation between experimental and DFT-calculated vibrational modes

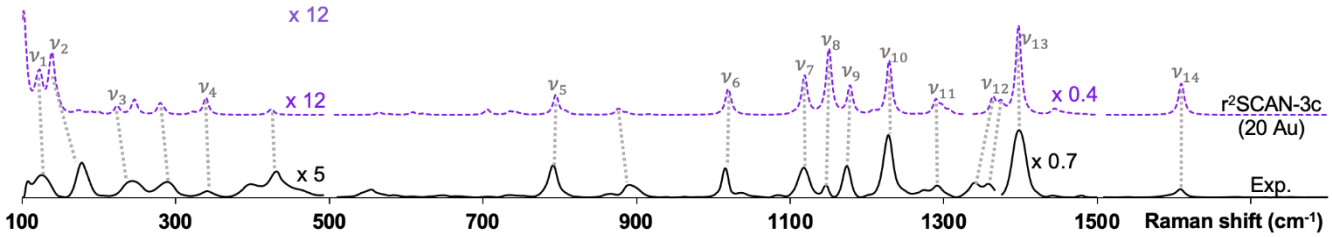
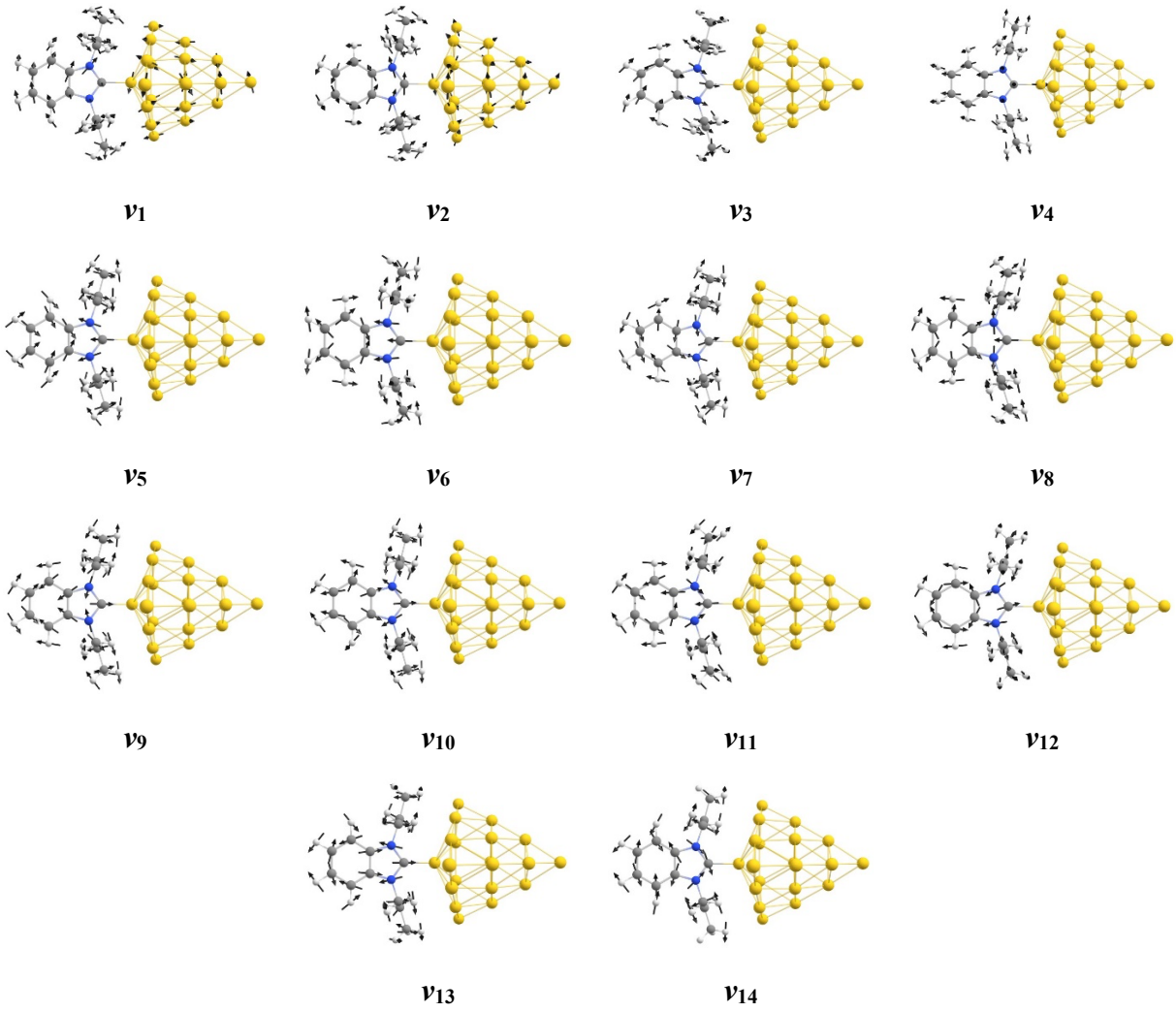


Figure S7. Experimental and predicted (r^{2}SCAN-3c TightOpt TightSCF) Raman spectrum of **C_3NHC-AuNP** in the 100-1700 cm^{-1} region



1.8. Relative Energies for C_{12}NHC complexes and nanoparticles

Table S8. Relative energies for different geometries of **C_{12}NHC-AuBr**

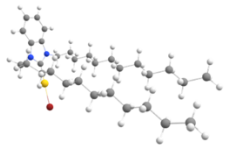
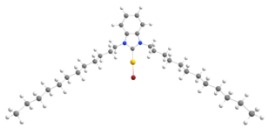
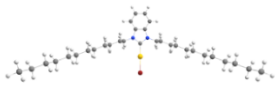
	Crystal structure	'Side' chains	'Up' chains
Relative energy, ΔG (kcal/mol)	0.00	2.59	2.59
Geometry (after optimization)			

Table S9. Relative energies for different geometries of **C_{12}NHC-AuNP**

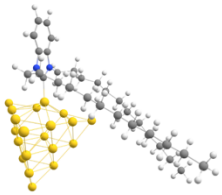
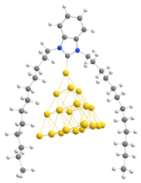
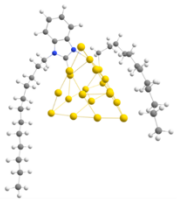
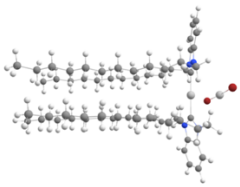
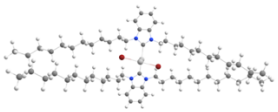
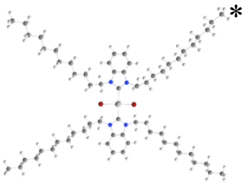
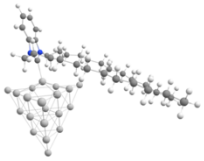
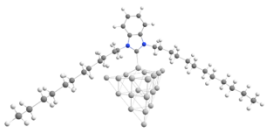
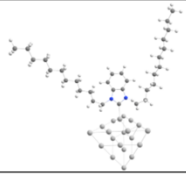
	Crystal structure	'Side' chains	'Up' chains
Relative energy, ΔG (kcal/mol)	0.00	21.43	17.23
Geometry (after optimization)			

Table S10. Relative energies for different geometries of **$[(C_{12}NHC)_2\text{-}Ag]^+$ $[AgBr_2]^-$**

	Crystal structure	'Side' chains	'Up' chains
Relative energy, ΔG (kcal/mol)	0.00	5.58	*Optimization didn't converge*
Geometry (after optimization)			 *

*Input geometry (before optimization)

Table S11. Relative energies for different geometries of **C_{12}NHC-AgNP**

	Crystal structure	'Side' chains	'Up' chains
Relative energy, ΔG (kcal/mol)	0.00	3.36	*Optimization didn't converge*
Geometry (after optimization)			 *

*Input geometry (before optimization)

III. Raman spectra

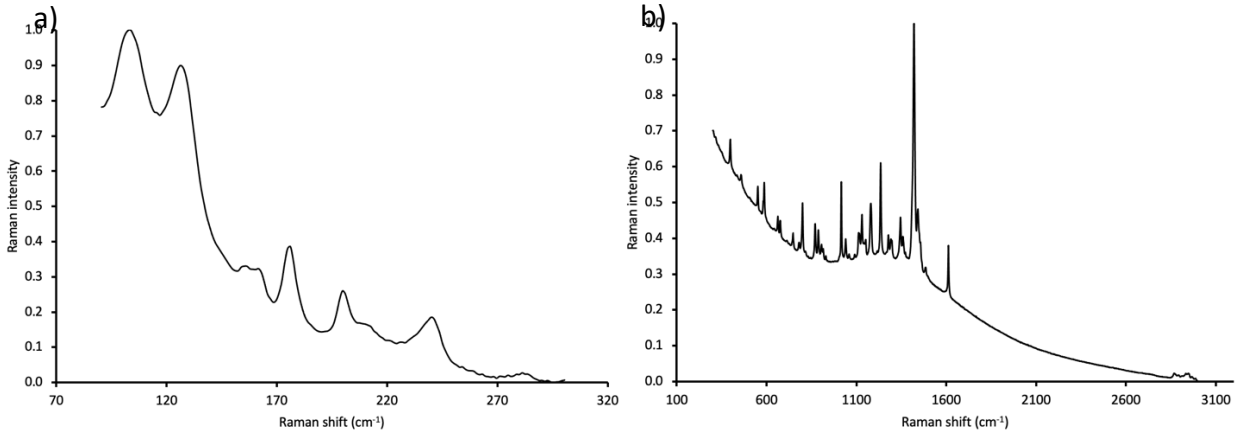


Figure S8. Normalized Raw Raman spectrum of **C_3NHC-AuBr** from a) 90 to 300 cm^{-1} and from b) 300 to 3100 cm^{-1} using a 785 nm laser excitation.

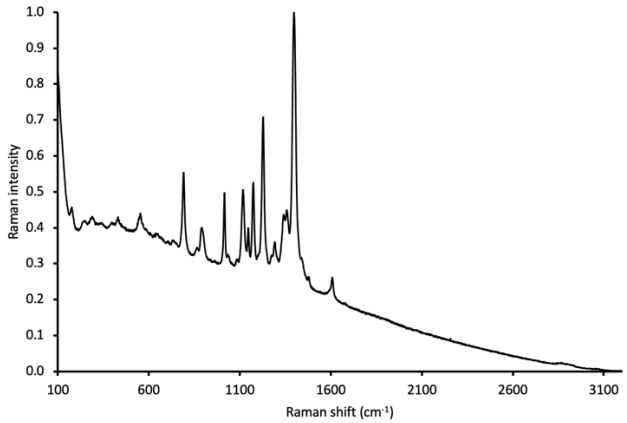


Figure S9. Normalized Raw Raman spectrum of **C_3NHC-AuNP** using a 785 nm laser excitation.

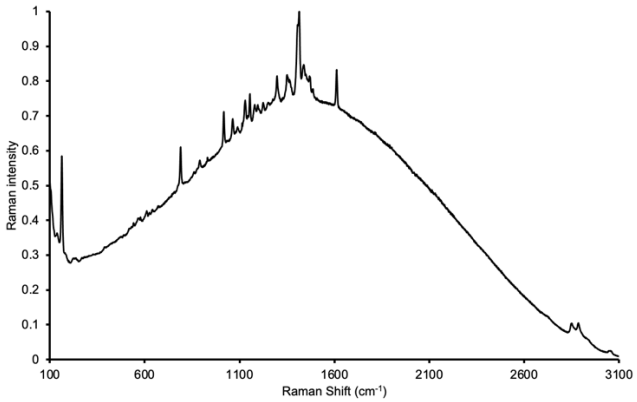


Figure S10. Raw Raman spectrum of **$[(C_{12}NHC)_2\text{-}Ag]^+$ $[AgBr_2]^-$** using a 785 nm laser excitation.

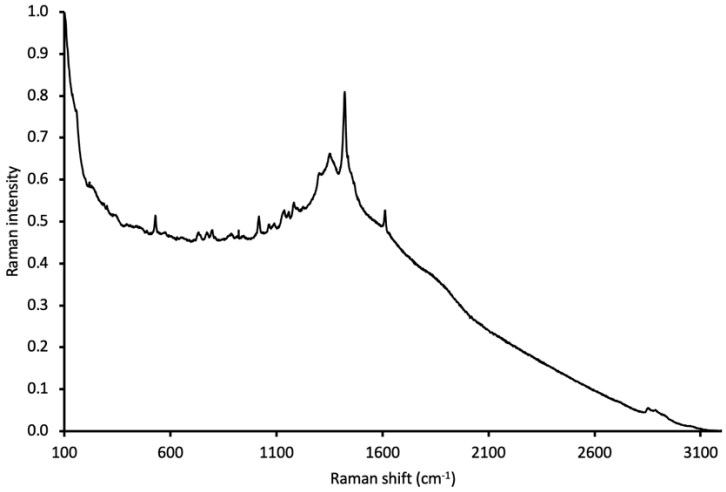


Figure S11. Raw Raman spectrum of **C_{12}NHC-AgNP** using a 532 nm laser excitation.

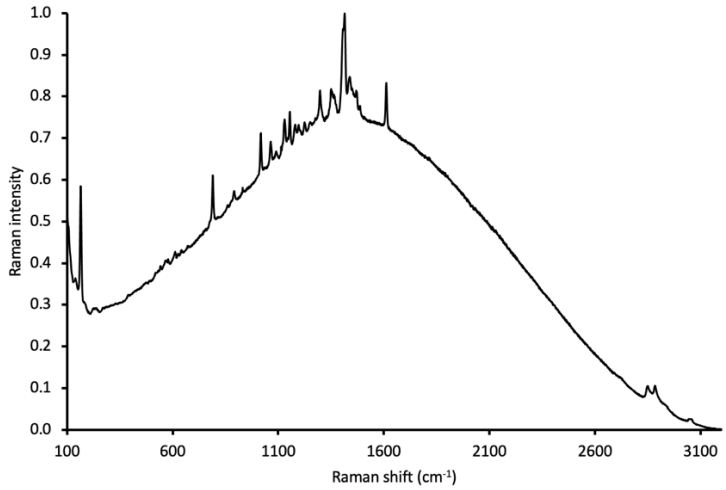


Figure S12. Raw Raman spectrum of **C_{12}NHC-AuBr** using a 785 nm laser excitation.

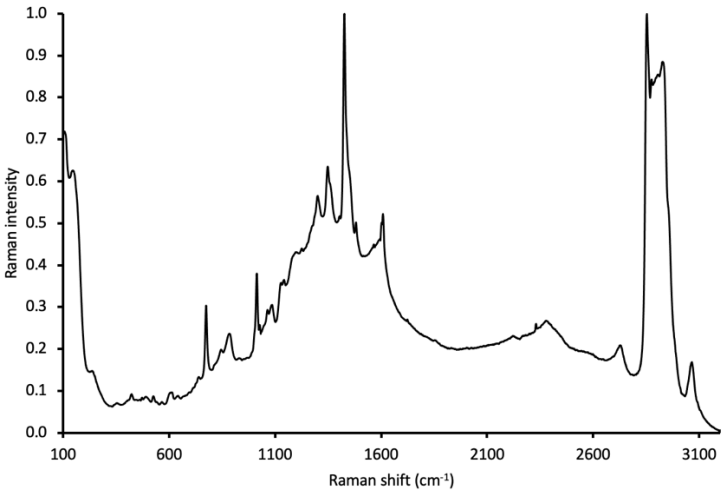


Figure S13. Raw Raman spectrum of **C_{12}NHC-AuNP** using a 785 nm laser excitation.

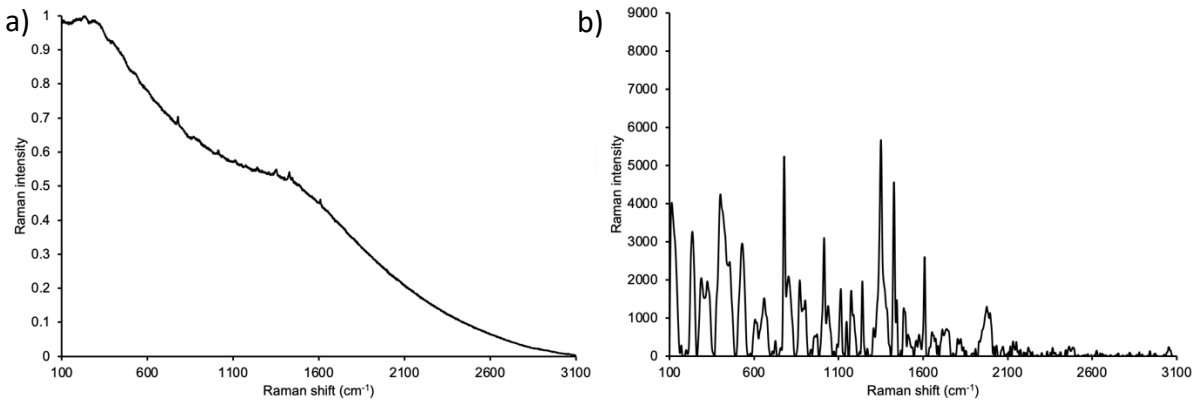


Figure S14. a) Raw Raman spectrum and b) corrected Raman spectrum of **3 (C_{12}NHC-H^+ Br^-)** using 785 nm laser excitation.

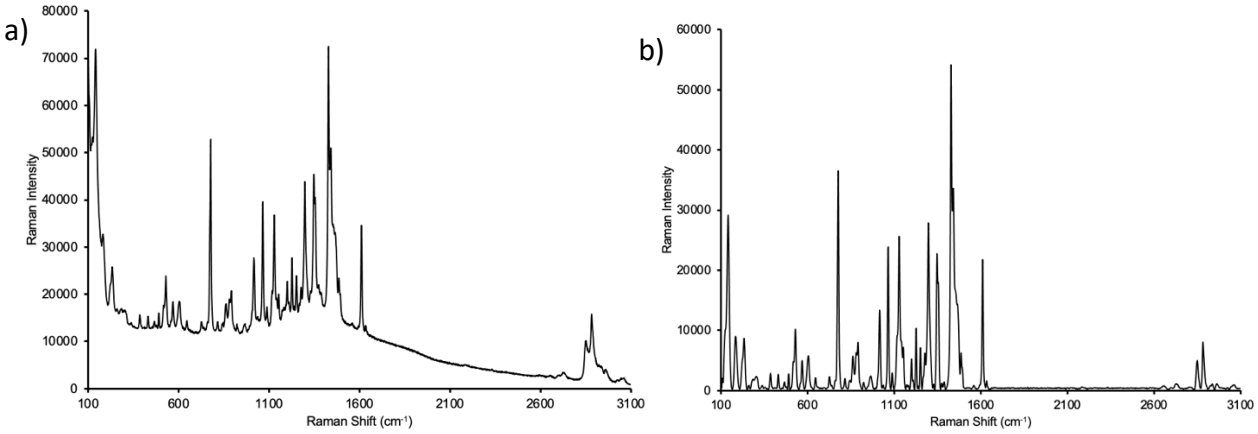


Figure S15. a) Raw and b) corrected Raman spectrum of **(C_3NHC-H^+ Br^-)** using 785 nm laser excitation.

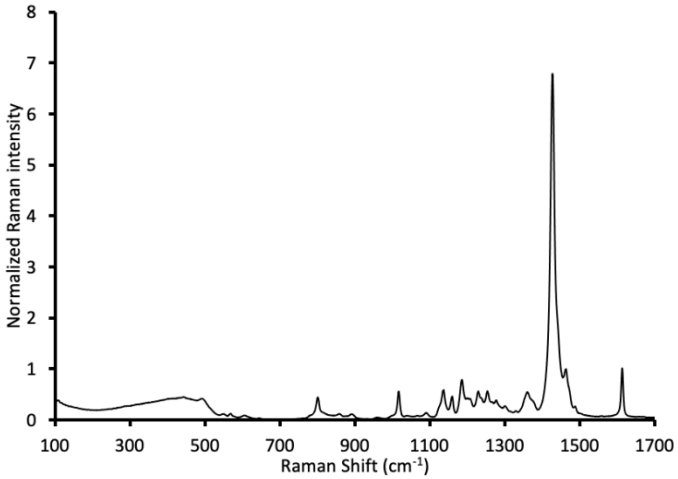


Figure S16. Raw Raman spectrum of C_{12}NHC-AuNP as a solid after dialyze in THF using 532 nm (5%) laser excitation

IV. UV-Vis Spectra

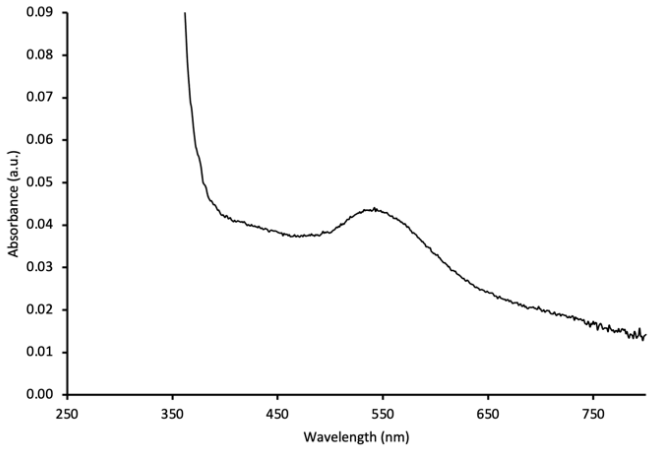


Figure S17. **C_{12}NHC-AuNP** UV-Vis Spectrum (2 mg/mL in THF)

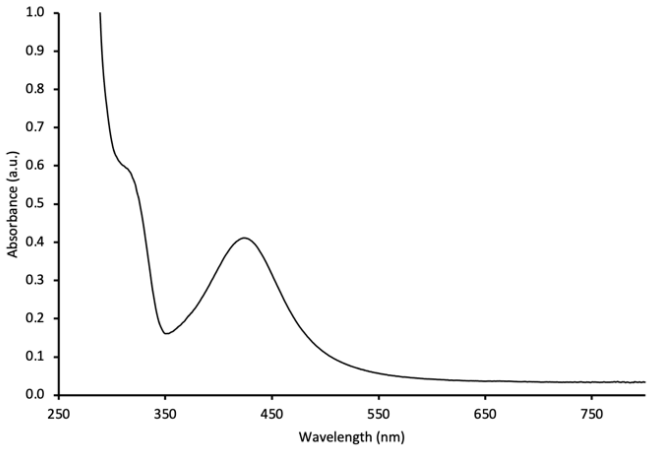


Figure S18. C_{12}NHC-AgNP UV-Vis Spectrum (0.45 mg/mL in THF)

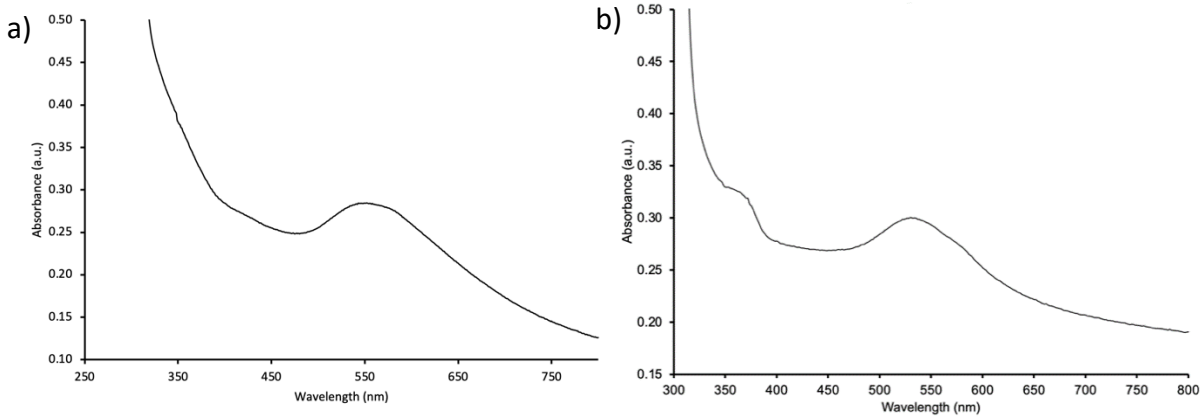


Figure S19. C_3NHC-AuNP UV-Vis Spectrum a) after the synthesis and b) 2 days after the synthesis (0.8 mg/mL in THF)

V. XRD Data

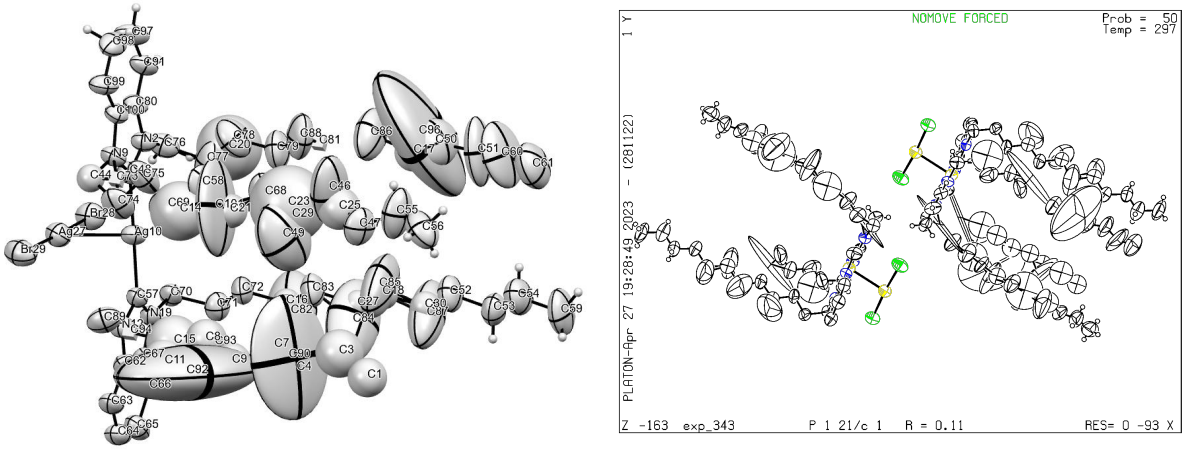


Figure S20. ORTEP structures of $[(C_{12}NHC)_2\text{-}Ag]^+ [AgBr_2]^-$

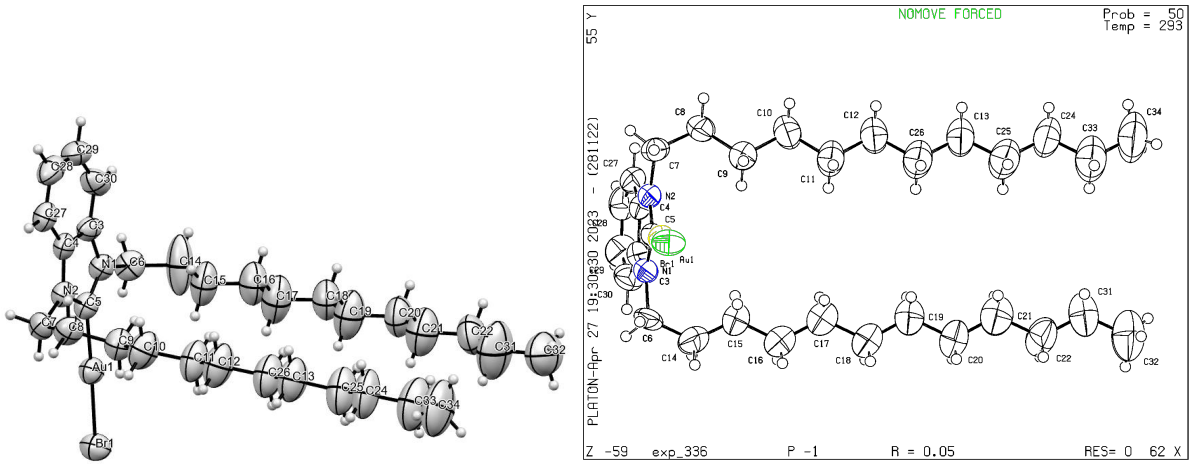


Figure S21. ORTEP structures of C_{12}**NHC-AuBr**

VI. NMR Data

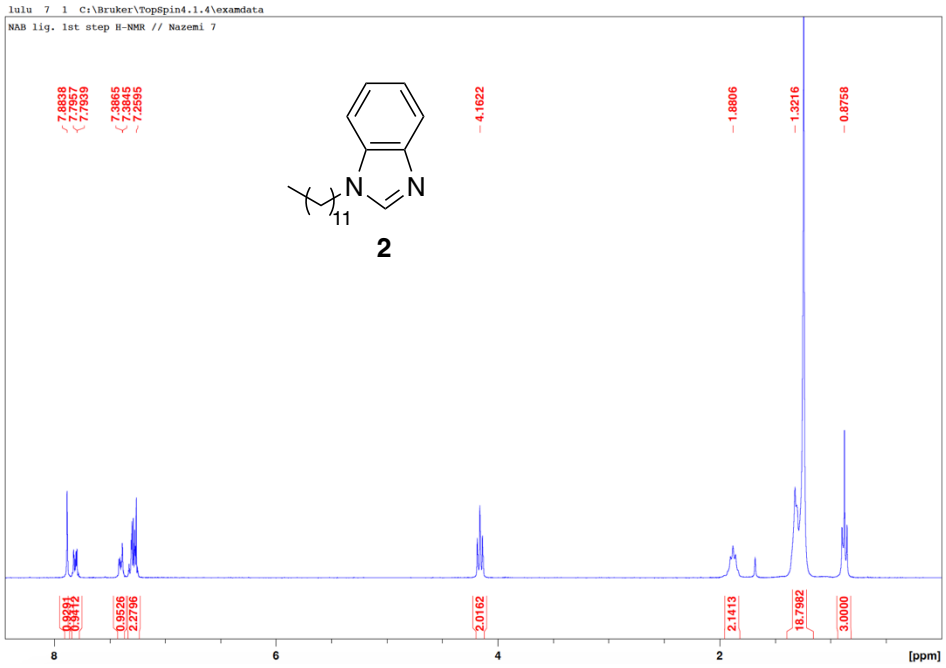


Figure S22. H^1 NMR spectrum of compound **2** (300 MHz, $CDCl_3$)

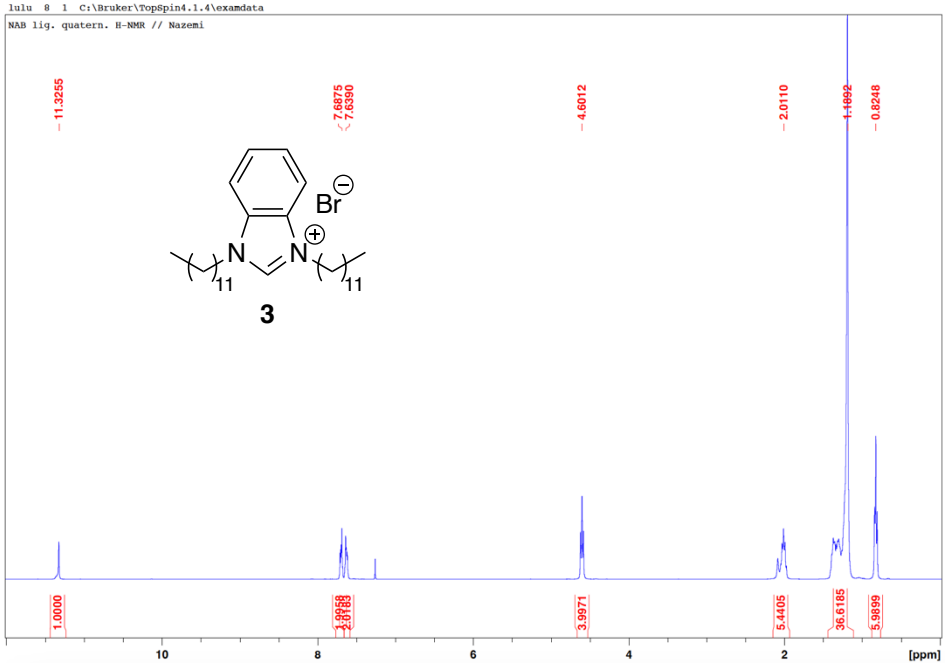


Figure S23. H^1 NMR spectrum of compound **3** H^1-NMR (300 MHz, $CDCl_3$)

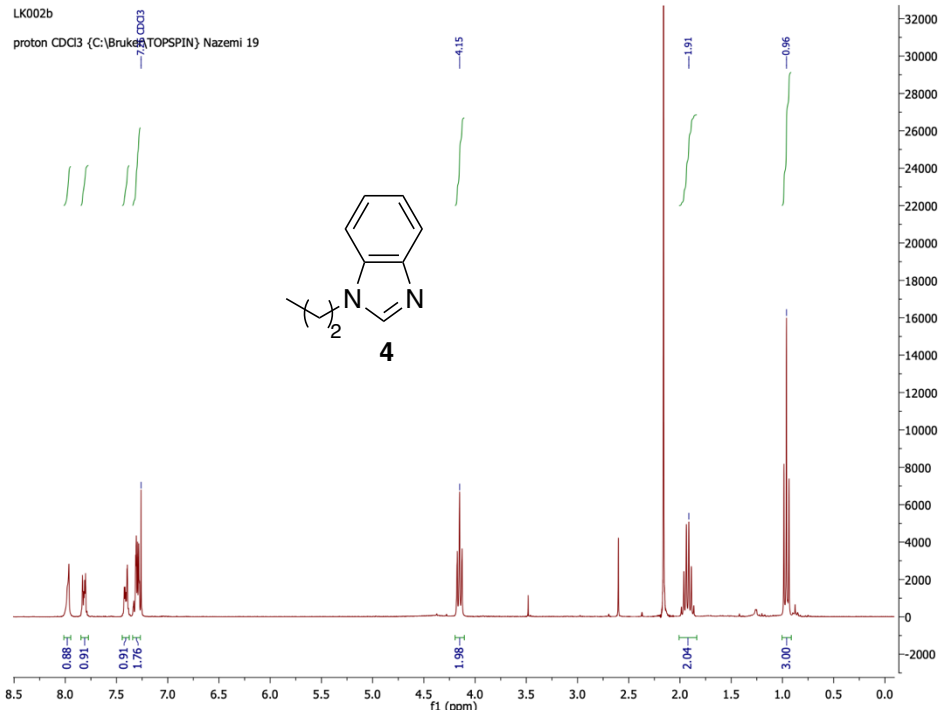


Figure S24. H^1 NMR spectrum of compound **4** (300 MHz, $CDCl_3$)

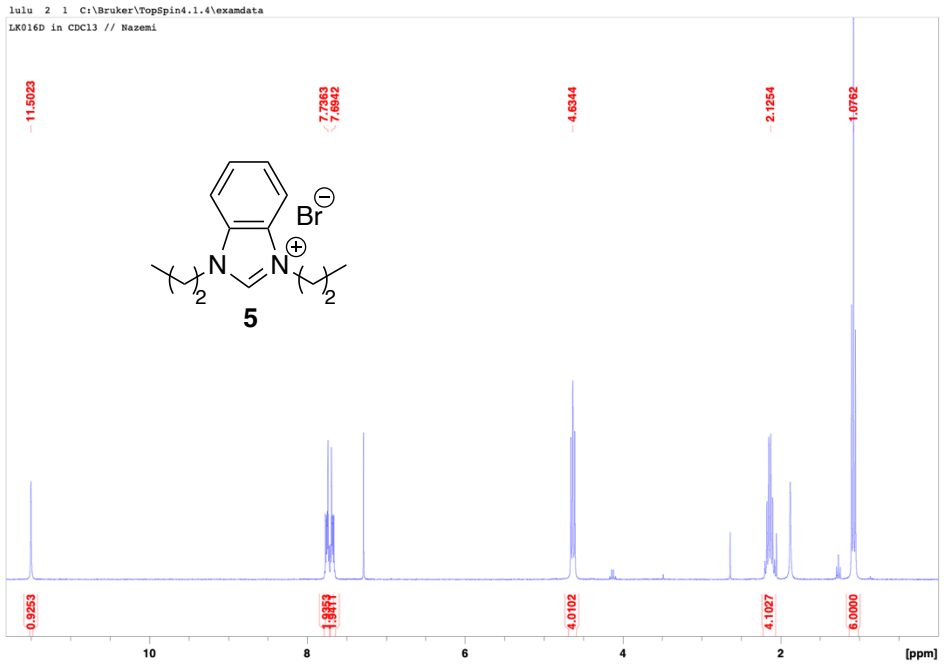


Figure S25. H^1 NMR spectrum of compound **5** (300 MHz, $CDCl_3$)

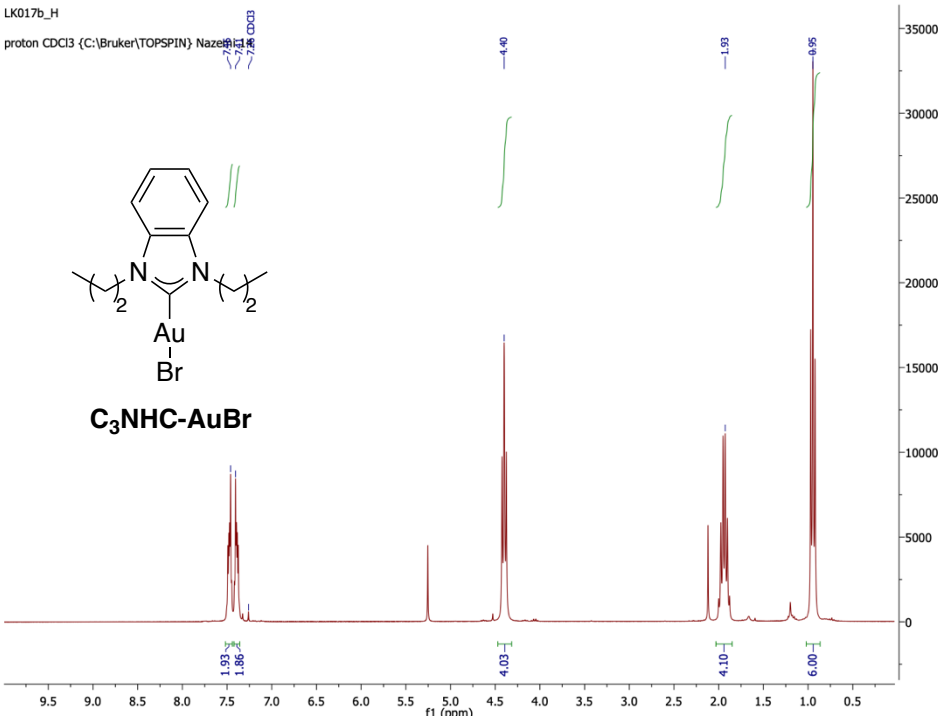


Figure S26. H^{1} NMR spectrum of **C_3NHC-AuBr** (300 MHz, $CDCl_3$)

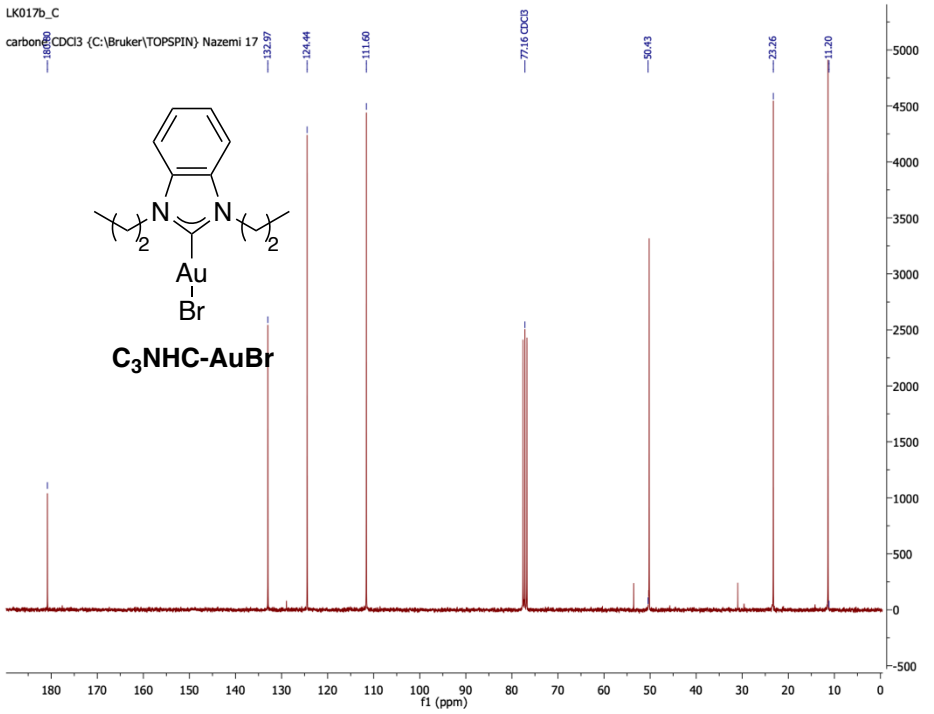


Figure S27. C^{13} NMR spectrum of **C_3NHC-AuBr** (300 MHz, $CDCl_3$)

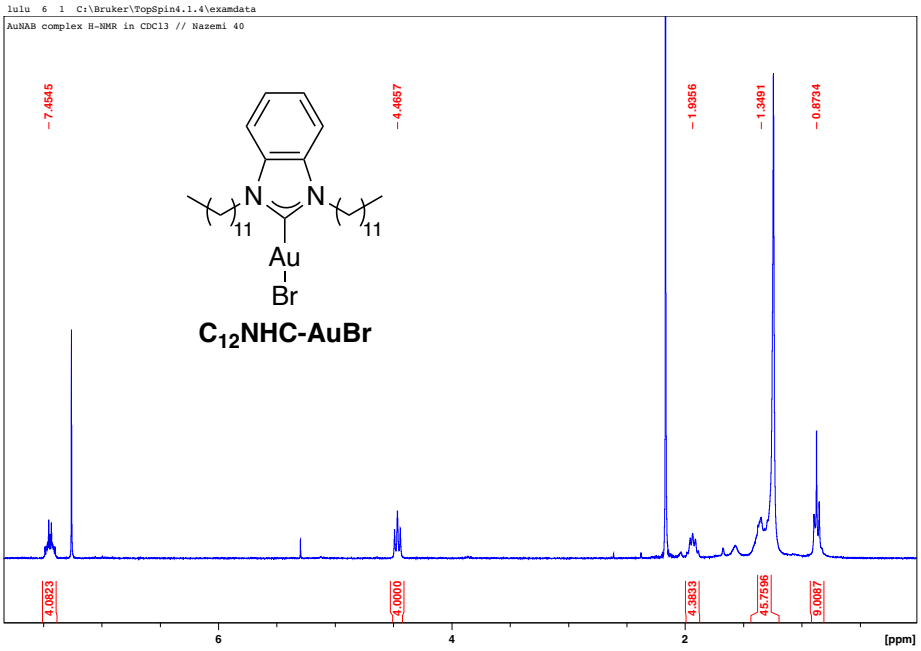


Figure S28. H^1 NMR spectrum of compound **C_{12}NHC-AuBr** (300 MHz, $CDCl_3$)

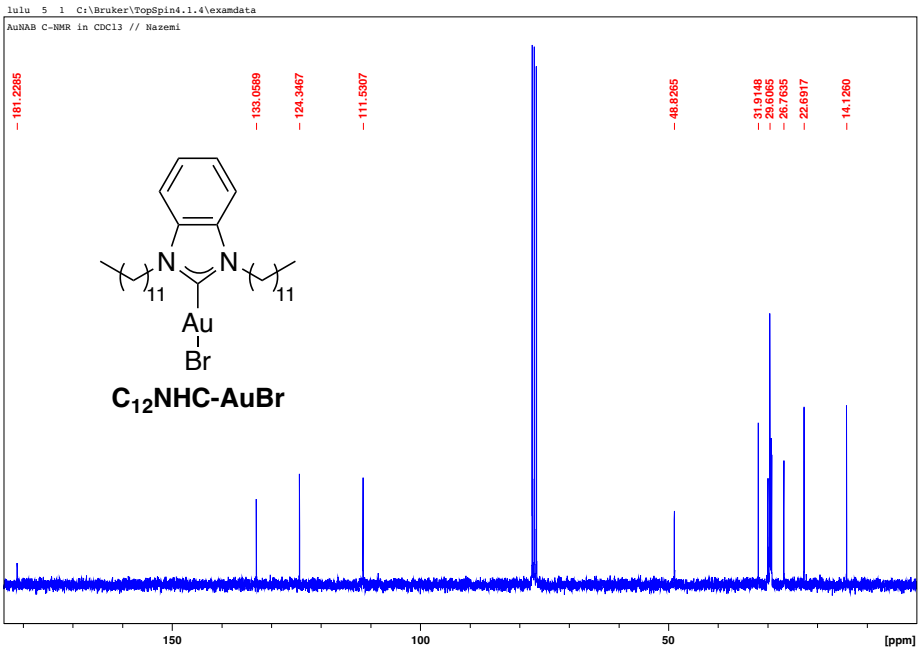


Figure S29. C^{13} NMR spectrum of compound **C_{12}NHC-AuBr** (300 MHz, $CDCl_3$)

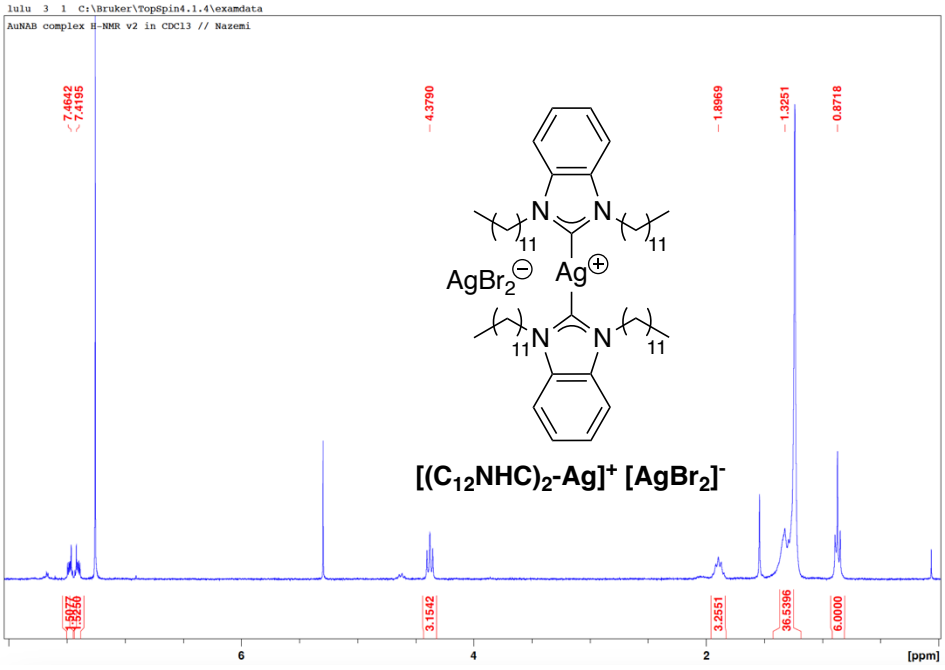


Figure S30. H^1 NMR spectrum of **$[(C_{12}NHC)_2\text{-}Ag]^+$ $[AgBr_2]^-$** (300 MHz, $CDCl_3$)

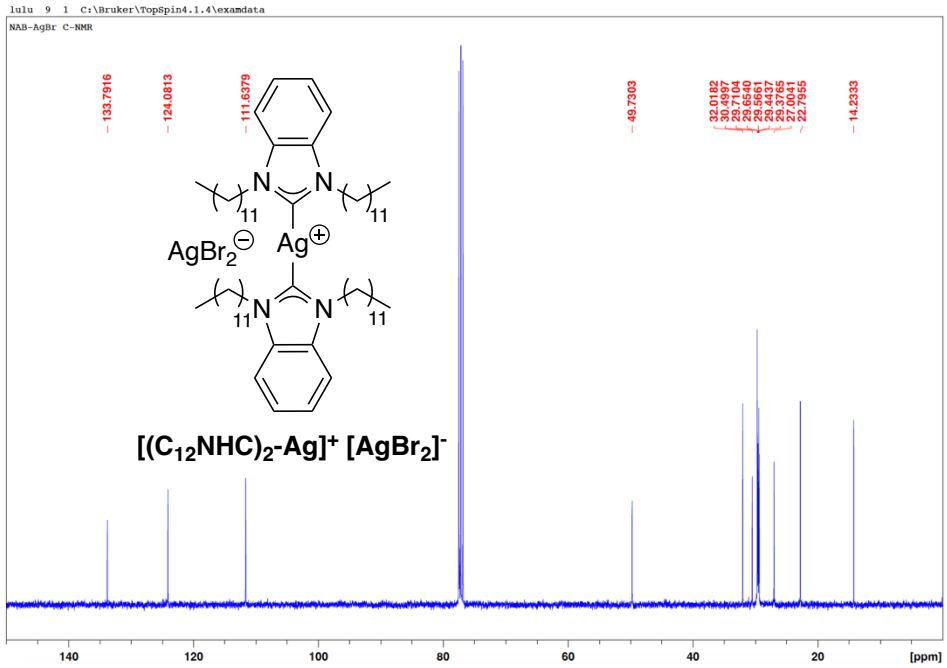


Figure S31. C^{13} NMR spectrum of **$[(C_{12}NHC)_2\text{-}Ag]^+$ $[AgBr_2]^-$** (300 MHz, $CDCl_3$)