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Supporting Information

# "Visualizing" the partially reversible conversion of gold nanoclusters *via* $Au_{23}(S\text{-}c\text{-}C_6H_{11})_{17}$ intermediate

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## I. Experimental section

### 1.1.Materials

All chemicals were purchased commercially and were used without prior purification. Tetrachloroauric (III) acid ($HAuCl_4$. $3H_2O$, > 99.9% metals basis), tetraoctylammonium bromide (TOAB, ≥ 98%), cyclohexane thiol (S-*c*-$C_6H_{11}$; 97%), sodium borohydride ($NaBH_4$, 99.99%, trace metal basis), trans-2-[3-(4-tert-butylphenyl)-2-methyl-2 propenylidene] malononitrile (DCTB, > 99.0%) were purchased from Sigma-Aldrich. MeOH (HPLC grade, 99.9%, Spectrochem), toluene (HPLC grade, 99.9%, Spectrochem), Dimethylene chloride (DCM, HPLC grade, 99.9%, Spectrochem), Tetrahydrofuran (THF, HPLC grade, 99.9%, Spectrochem), 4-Flurothiophenol (*p*-$FC_6H_4SH$; 98%), 4-Chlorothiophenol (*p*-$ClC_6H_4SH$; 97%), 4-Bromothiophenol (*p*-$BrC_6H_4SH$; 95%), Thiophenol ($C_6H_5SH$; 97%), PTFE syringe filters (0.2 µm, Corning, Germany) and BioBeads S- X1 (BioRad) were used as purchased. The water used in all experiments was ultrapure (resistivity: 18.2 MΩ cm), produced by a Milli-Q NANO pure water system. All glassware was thoroughly cleaned with aqua regia (HCl: $HNO_3$= 3:1, v: v) and rinsed with abundant pure water.

### 1.2. Methods

**Synthesis of $[Au_{23}(S\text{-}c\text{-}C_6H_{11})_{16}]^-$ nanocluster.** The synthesis of $[Au_{23}(S\text{-}c\text{-}C_6H_{11})_{16}]^-$ was conducted as per the previously reported method.[19] Firstly, $HAuCl_4$. $3H_2O$ (0.6 mmol, 236.3 mg) and tetraoctylammonium bromide (TOAB, 0.696 mmol, 380 mg) were dissolved in 30 mL of methanol in a 50 mL tri-necked round-bottom flask. The color of the solution changed from yellow to dark reddish-orange upon vigorous stirring for 15 min. To this solution, an excess of 1-cyclohexanethiol was added (3.2 mmol, 390 µL) was added to the mixture at room temperature. The solution turned yellowish from reddish brown almost immediately, indicating the formation of Au(I) from Au(III) complexes. After 15 min, $NaBH_4$ (6 mmol, 227 mg dissolved freshly in 12 mL of cold nano pure water) was rapidly added to the solution under vigorous stirring. The formation of a black-colored solution indicated the formation of Au NCs, which was further precipitated out of the solution using methanol. The reaction mixture was further allowed to stir overnight which finally yielded the pure $[Au_{23}(S\text{-}c\text{-}C_6H_{11})_{16}]^-$ NC.

**Transformation of $[Au_{23}(S\text{-}c\text{-}C_6H_{11})_{16}]^-$ nanocluster using FBT:** 5 mg of $[Au_{23}(S\text{-}c\text{-}C_6H_{11})_{16}]^-$ was dissolved in 1 mL of dichloromethane and was centrifuged at (25 °C, 10000 rpm) for 10 minutes to remove any insoluble particles. 0.25 mL *p*-Flurothiophenol was added to the supernatant and heated at 40 °C. The reaction was continued for two hours. Small aliquots were taken from the reaction mixture for the UV-Vis spectroscopy and MALDI-MS measurements. The obtained product was purified using size-exclusion chromatography (SEC), filtered using a 0.2 µm PTFE syringe filter, and dried using rotavapor. Single crystals of the as-prepared NCs were obtained by layering the DCM solution of NCs with hexane in less than a week at room temperature.

**Transformation of $[Au_{23}(S\text{-}c\text{-}C_6H_{11})_{16}]^-$ nanocluster using CBT/ BBT:** 5 mg of $[Au_{23}(S\text{-}c\text{-}C_6H_{11})_{16}]^-$ was dissolved in 1 mL of dichloromethane and was centrifuged at (25 °C, 10000 rpm) for 10 minutes to remove any insoluble particles. 290 mg *p*-chlorothiophenol/ 378 mg *p*-bromothiophenol was added to the supernatant and heated at 40 °C. The reaction was continued for three hours. Small aliquots were taken from the reaction mixture for the UV-Vis spectroscopy and MALDI-MS measurements. The obtained product was purified using size-exclusion chromatography (SEC), filtered using a 0.2 µm PTFE syringe filter, and dried using rotavapor. Single crystals of the as-prepared NCs were obtained by layering the DCM solution of NCs with hexane in less than a week at room temperature.

## II. Characterization

The absorption spectra were obtained on a UV-3800 SHIMADZU UV-Vis NIR spectrometer using dichloromethane as a solvent. The mass spectra of the NC samples were acquired by using a Brucker Microflex MALDI-TOF mass spectrometer. DCTB was used as a matrix and the sample was prepared as 1 mg in 100 µL of dichloromethane for the same. From the stock solution, various amounts of the stock solution were taken and mixed with 1 µL of the analyte solution. The molecules were ionized with the Nd: YAG laser ($\lambda = 266$ nm). The analyte concentration was optimized to get a well-resolved spectrum. ESI mass spectra were recorded using a Waters Q-TOF mass spectrometer equipped with a Z-Spray source. The source temperature was kept at 70 ºC. The sample was directly infused into the chamber at 5 µL/min. The spray voltage was kept at 3.0 kV and the cone voltage at 30 V. To prepare the ESI sample, clusters were dissolved in dichloromethane (1 mg/ mL) and diluted (2: 1 v) using methanol solvent. Femtosecond transient absorption measurements were conducted by dissolving the NCs in DCM and exciting with a 400

nm pump with a fluence of 490 nJ/cm² and a white light probe (500-730 nm) was used to measure the absorption in the excited state.

### 2.1 Single Crystal X-Ray Diffraction

The single crystal of $Au_{25}(FC_6H_4S)_{18}$ with dimensions of 0.125 mm x 0.225 mm x 0.288 mm was mounted on Bruker D8 Quest - Microfocus SCXRD (single crystal X-ray diffractometer) with Bruker PHOTON III C14, CPAD detector using MoKα radiation (λ= 0.71073 Å). The total exposure time for data collection was 1.87 hours. The frames were integrated with the Bruker SAINTS software package using a narrow-frame algorithm. The crystal structure was solved and refined by by SHELXTL software package.[S1, S2, S3, S4] The extra framework cation, tetraoctyl ammonium was not detected properly based on the single crystal data. However, we could identify it through ESI-MS data.

## III. Computational Details

The density functional theory (DFT) calculations were performed using Generalized gradient approximation as implemented in Perdew–Burke– Ernzerhof (PBE) functional with the help of Vienna Ab Initio Software Package (VASP).[S5, S6] To describe the electron-ion interactions projector augmented wave (PAW) method was employed along with an energy cutoff of 470 eV.[S7,S8] We have fit the nanocluster inside a 30 × 30 × 30 $Å^3$ cubic cell to avoid periodic interactions. A gamma-centered (1×1×1) k-point was used to sample the Brillouin zone. DFT-D3 dispersion correction as implemented by Grimme was used.[S9] The equations used for the calculation of cohesive energy of the core ($E_c$) and shell-to-core binding energy ($E_{SC}$) are as follows:

$$E_c = \frac{E_{cluster} - n \times E_{Au} - E_{shell}}{n + n_{shell-int}}$$

$$E_{sc} = \frac{E_{cluster} - E_{core} - E_{shell}}{n_{shell-int}}$$

Where $E_{cluster}$ is the total energy of the cluster, $E_{Au}$ is the energy of a single gold atom, $E_{core}$ is the energies of gold core and $E_{shell}$ is the single point energies of the surrounding shell at the optimized geometries of the clusters, n is the number of core gold atoms and $n_{shell-int}$ is the number of shell units interacting with the core.

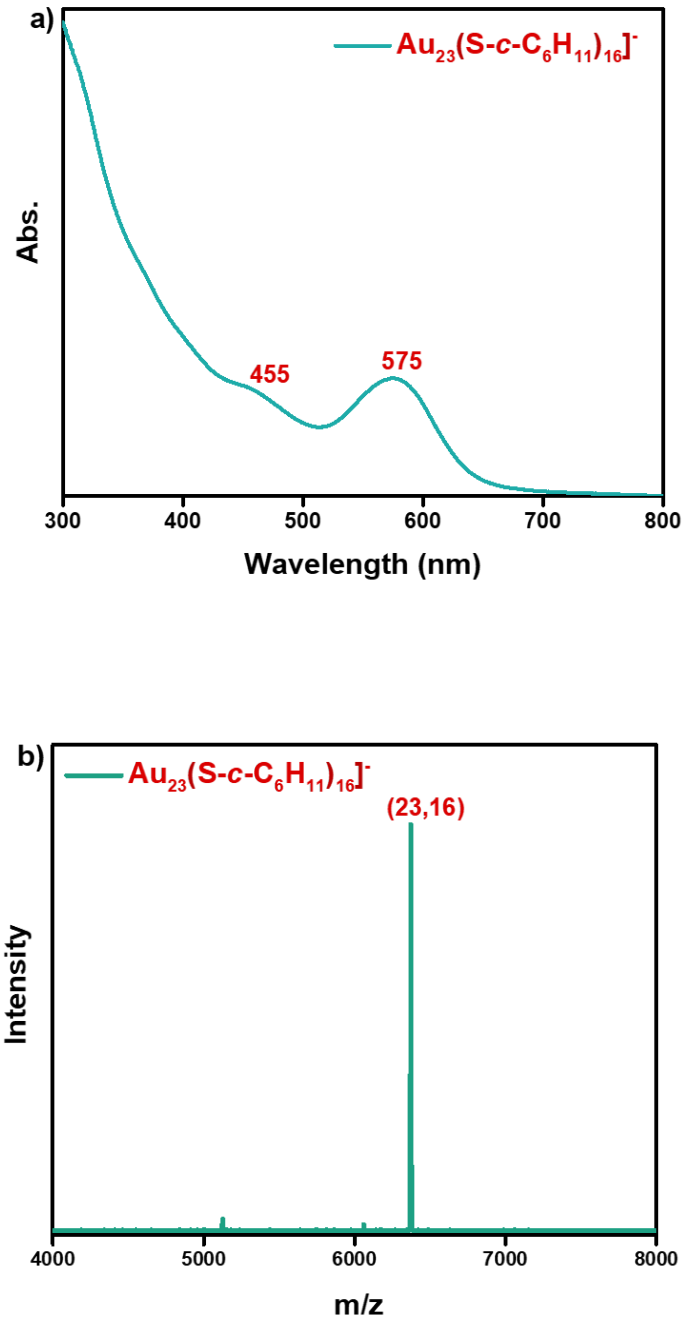
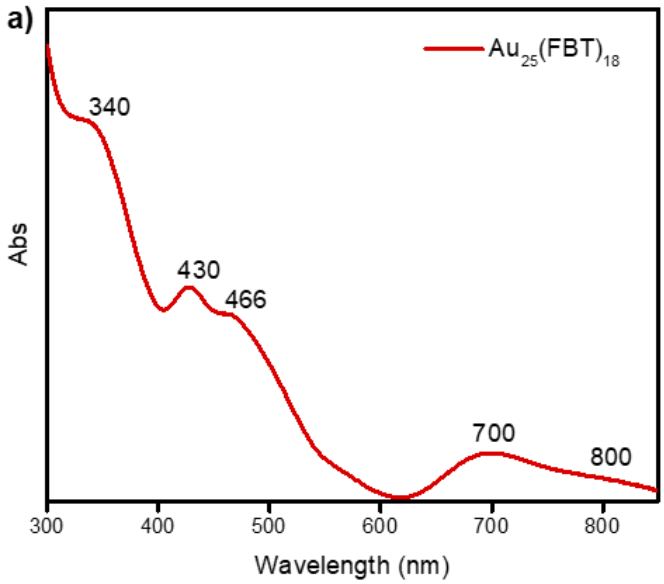
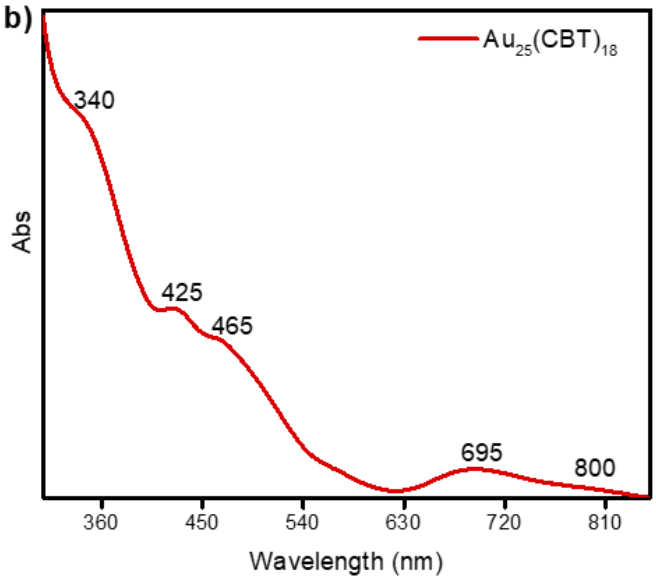



**Figure S1.** a) UV-vis absorption spectrum and b) MALDI-MS spectrum of the synthesized $[Au_{23}(S\text{-}c\text{-}C_6H_{11})_{16}]^-$ NC.


a)
Au25(FBT)18
340
430
466
700
800
Abs
300
400
500
600
700
800
Wavelength (nm)


b)
Au25(CBT)18
340
425
465
695
800
Abs
360
450
540
630
720
810
Wavelength (nm)

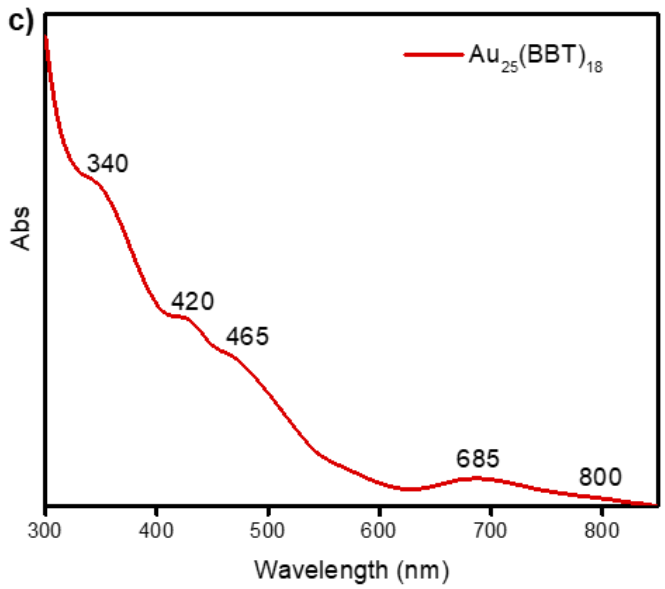
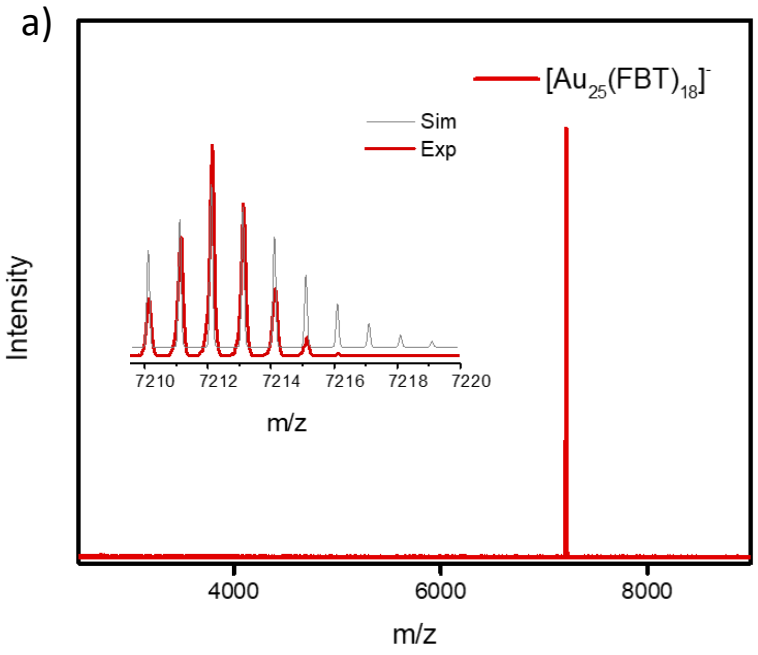
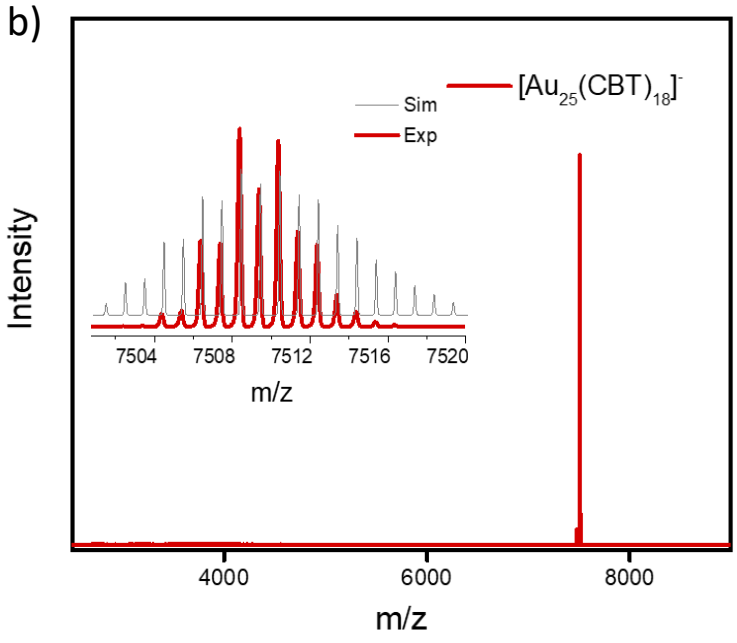



**Figure S2.** UV-vis absorption spectra of a) $[Au_{25}(FBT)_{18}]^-$, b) $[Au_{25}(CBT)_{18}]^-$ and c) $[Au_{25}(BBT)_{18}]^-$ NCs.


a)
[Au25(FBT)18]-
Sim
Exp
Intensity
7210
7212
7214
7216
7218
7220
m/z
4000
6000
8000
m/z


b)
[Au25(CBT)18]-
Sim
Exp
Intensity
7504
7508
7512
7516
7520
m/z
4000
6000
8000
m/z

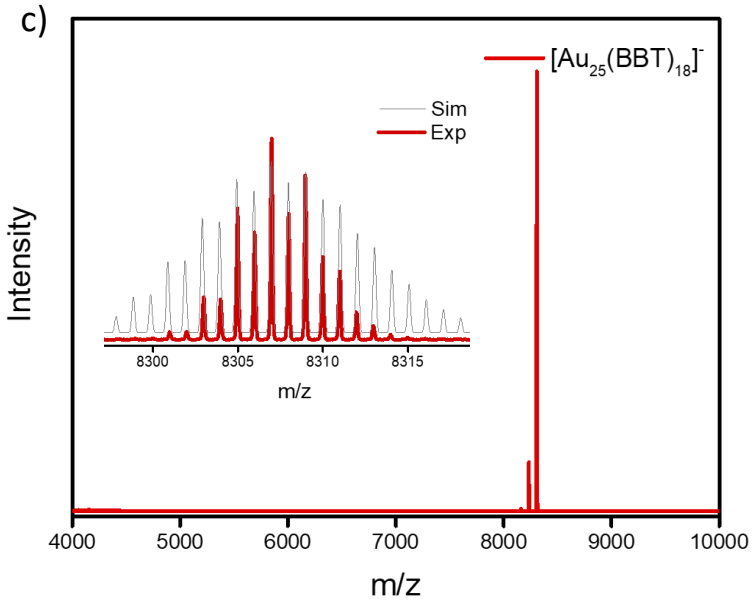



**Figure S3.** Negative-ion mode ESI mass spectra of a) $[Au_{25}(FBT)_{18}]^-$, b) $[Au_{25}(CBT)_{18}]^-$, and c) $[Au_{25}(BBT)_{18}]^-$ NCs. The inset shows the respective experimental and simulated isotopic patterns.

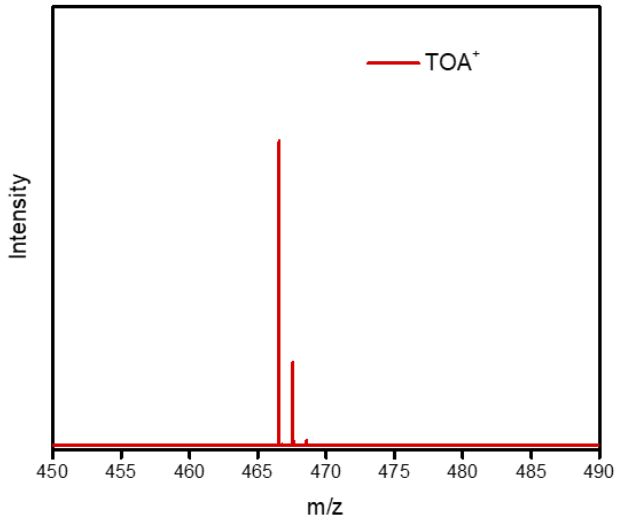



**Figure S4.** Positive-ion mode ESI mass spectra of $[Au_{25}(XBT)_{18}]^-$ NCs showing the presence of $TOA^+$ counter cation.

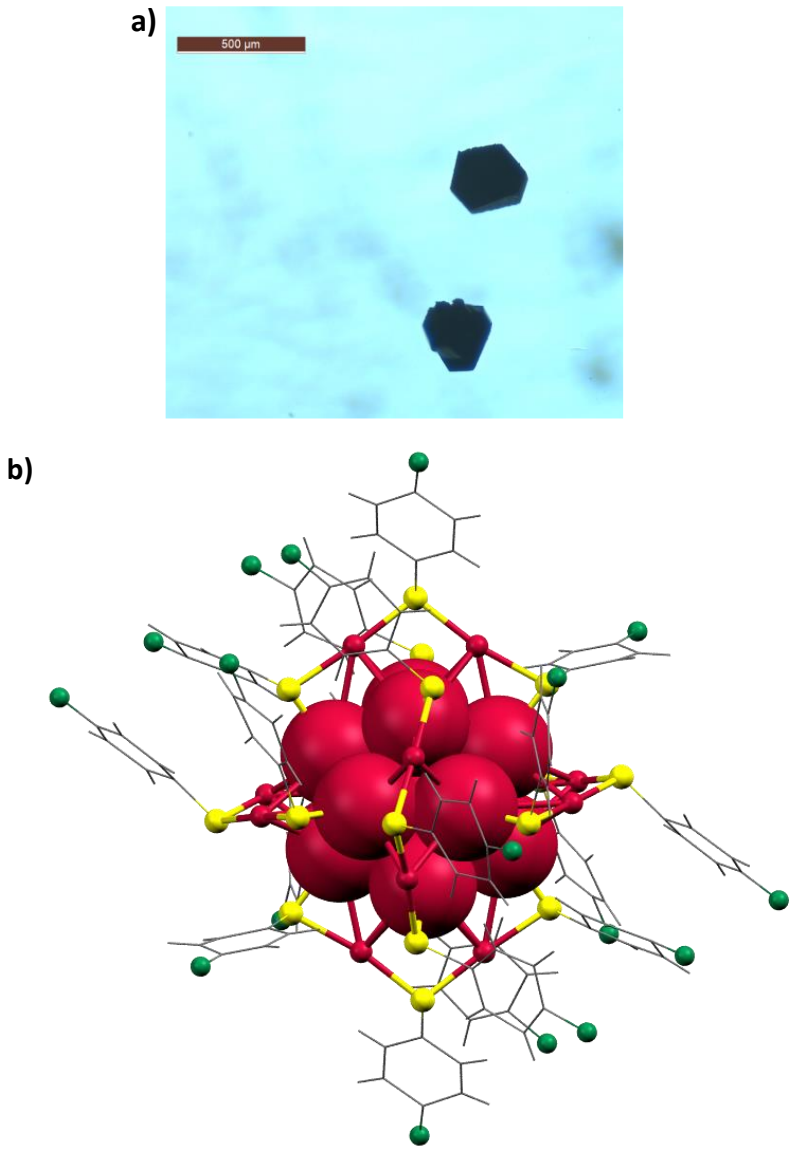



**Figure S5.** a) Optical microscope image of the single crystals of $Au_{25}(FBT)_{18}$ NC. b) Total structure of the $[Au_{25}(FBT)_{18}]^-$ NC. Color legend: red sphere, Au; yellow sphere, S; green sphere, F; grey stick, C and H.

**Table S1**. Crystal structure refinement parameters of $[Au_{25}(FBT)_{18}]^-$ NC.

| | |
|---|---|
| Identification code | 0061_260324_SG53A |
| Empirical formula | C108 H72 Au25 F18 S18 |
| CCDC number | 2334107 |
| Formula weight | 7212.89 g/mol |
| Temperature/K | 100 |
| Wavelength/Å | 0.71073 |
| Crystal system | Monoclinic |
| Space group | *C2/c* (No. 15) |
| a/Å | 29.6682(14) |
| b/Å | 17.7115(9) |
| c/Å | 34.7181(18) |
| α/° | 90 |
| β/° | 114.038(2) |
| γ/° | 90 |
| Volume/$Å^3$ | 16661.1(15) |
| Z | 4 |
| $\rho_{calc}g/cm^3$ | 2.876 |
| $\mu/mm^{-1}$ | 22.190 |
| F(000) | 12580.0 |
| Crystal size/$mm^3$ | 0.125 × 0.225 × 0.288 |
| 2θ range for data collection/° | 2.08 to 25.03 |
| Index ranges | $-35 \leq h \leq 32$, $-21 \leq k \leq 21$, $-41 \leq l \leq 41$ |
| Reflections collected | 185497 |
| Independent reflections | 14690 [R(int) = 0.0498] |
| Data/restraints/parameters | 14690/80/791 |
| Goodness-of-fit on $F^2$ | 1.167 |
| Final R indexes [I>=2σ (I)] | $R_1 = 0.0610$, $wR_2 = 0.1451$ |
| Largest diff. peak/hole / e $Å^{-3}$ | 3.328 and -2.689 |

**Table S2**. Selected bond distances in $[Au_{25}(FBT)_{18}]^-$ NC.

| Atoms | Bond length (Å) |
|---|---|
| Au(01) – Au(6A) | 2.7534(8) |
| Au(01) – Au(6A) | 2.7534(8) |
| Au(01) – Au(03) | 2.7596(7) |
| Au(01) – Au(03) | 2.7596(7) |
| Au(01) – Au(04) | 2.7790(8) |
| Au(01) – Au(04) | 2.7790(8) |
| Au(01) – Au(2A) | 2.7923(7) |
| Au(01) – Au(2A) | 2.7923(7) |
| Au(01) – Au(07) | 2.7934(8) |
| Au(01) – Au(07) | 2.7934(8) |
| Au(01) – Au(05) | 2.8106(7) |
| Au(01) – Au(05) | 2.8107(7) |
| Au(2A) – Au(03) | 2.8113(11) |
| Au(2A) – Au(07) | 2.9068(12) |
| Au(2A) – Au(6A) | 2.9334(11) |
| Au(2A) – Au(04) | 2.9498(11) |
| Au(2A) – Au(05) | 2.9873(11) |
| Au(2A) – Au(10) | 3.0754(12) |
| Au(2A) – Au(09) | 3.1011(11) |
| Au(2A) – Au(11) | 3.1864(11) |
| Au(6A) – Au(05) | 2.8110(10) |
| Au(6A) – Au(07) | 2.9563(11) |
| Au(6A) – Au(04) | 2.9639(11) |
| Au(6A) – Au(03) | 2.9825(11) |
| Au(6A) – Au(3C) | 3.0368(11) |
| Au(6A) – Au(10) | 3.0762(11) |
| Au(6A) – Au(13) | 3.1576(11) |
| Au(3C) – Au(05) | 3.1574(11) |
| Au(3C) – Au(07) | 3.1819(11) |
| Au(2B) – Au(10) | 2.20(5) |
| Au(2B) – Au(6B) | 2.50(5) |
| Au(2B) – Au(03) | 2.55(4) |
| Au(2B) – Au(09) | 3.11(4) |
| Au(2B) – Au(04) | 3.29(4) |
| Au(6B) – Au(13) | 2.46(4) |
| Au(6B) – Au(04) | 2.51(4) |
| Au(6B) – Au(3D) | 2.75(6) |
| Au(6B) – Au(05) | 3.14(4) |
| Au(6B) – Au(10) | 3.21(4) |
| Au(3D) – Au(05) | 2.23(4) |

| | |
|---|---|
| Au(3D) – Au(07) | 2.60(4) |
| Au(3D) – Au(13) | 3.06(4) |
| Au(03) – Au(04) | 2.8924(11) |
| Au(03) – Au(05) | 2.9065(11) |
| Au(03) – Au(07) | 3.0674(11) |
| Au(03) – Au(09) | 3.1089(11) |
| Au(03) – Au(08) | 3.1211(11) |
| Au(03) – Au(10) | 3.1220(11) |
| Au(04) – Au(07) | 2.8334(11) |
| Au(04) – Au(05) | 2.9886(11) |
| Au(04) – Au(11) | 3.0933(11) |
| Au(04) – Au(13) | 3.1515(11) |
| Au(04) – Au(08) | 3.1746(11) |
| Au(05) – Au(07) | 2.8910(11) |
| Au(05) – Au(13) | 3.0976(11) |
| Au(05) – Au(09) | 3.1894(11) |
| Au(07) – Au(08) | 3.0335(11) |
| Au(07) – Au(11) | 3.1132(11) |
| Au(6A) – S(01) | 2.410(5) |
| Au(3C) – S(06) | 2.298(6) |
| Au(3C) – S(03) | 2.316(6) |
| Au(2B) – S(08) | 2.51(4) |
| Au(6B) – S(01) | 2.24(4) |
| Au(3D) – S(06) | 2.53(4) |
| Au(3D) – S(03) | 2.66(4) |
| Au(3D) – S(02) | 2.412(5) |
| Au(04) – S(09) | 2.385(5) |
| Au(05) – S(04) | 2.396(5) |
| Au(07) – S(03) | 2.415(5) |
| Au(08) – S(05) | 2.319(5) |
| Au(08) – S(02) | 2.332(5) |
| Au(09) – S(07) | 2.304(6) |
| Au(09) – S(04) | 2.312(6) |
| Au(10) – S(07) | 2.297(5) |
| Au(10) – S(01) | 2.318(5) |
| Au(11) – S(08) | 2.289(6) |
| Au(11) – S(05) | 2.311(5) |
| Au(13) – S(06) | 2.294(6) |
| Au(13) – S(09) | 2.317(6) |

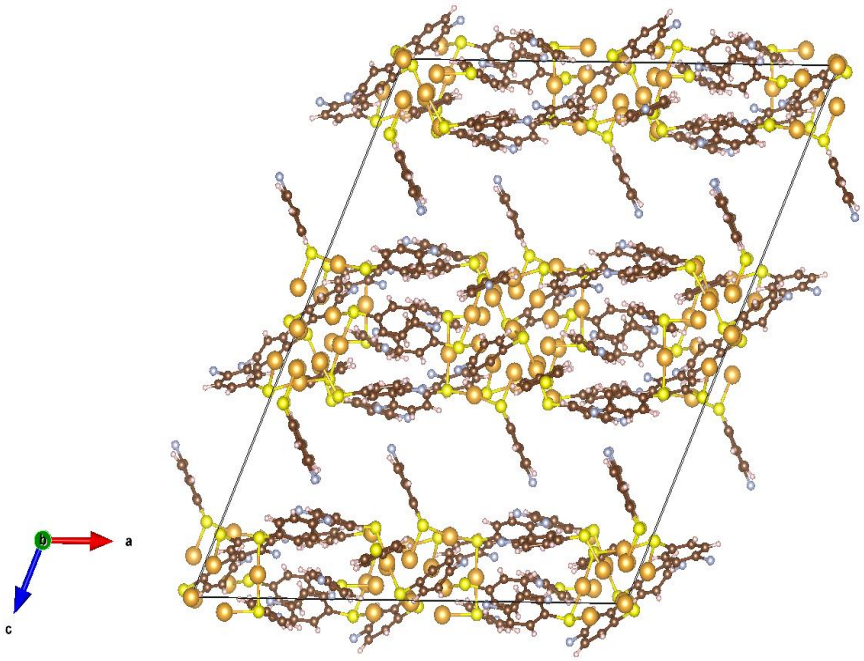
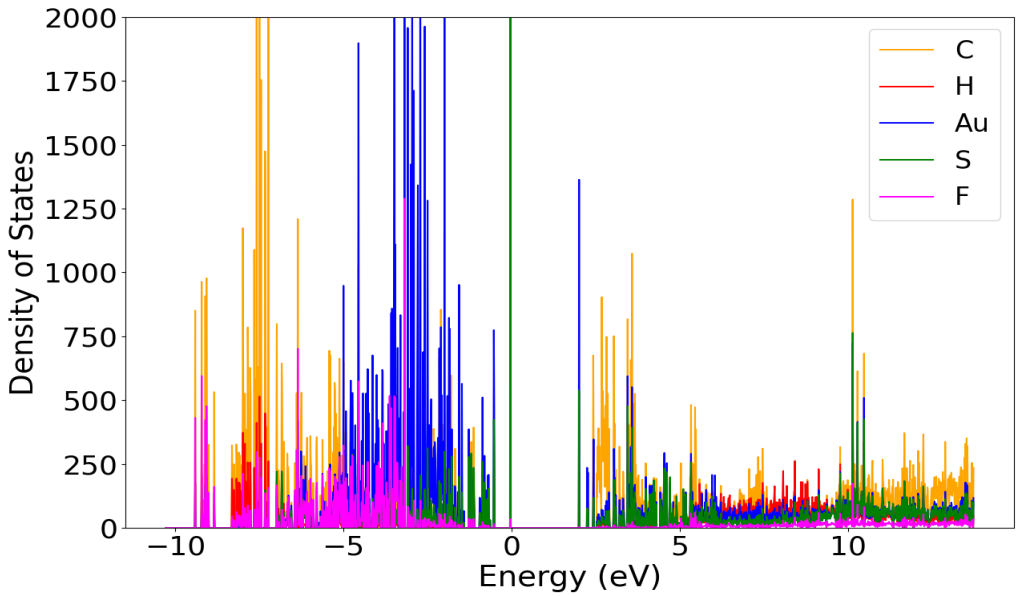



**Figure S6.** Relaxed structure of the $[Au_{25}(XBT)_{18}]^-$ NCs, X = F, Cl, Br. Color legend: Golden yellow, Au; yellow, S; Blue, F, Cl, Br; Brown, C.

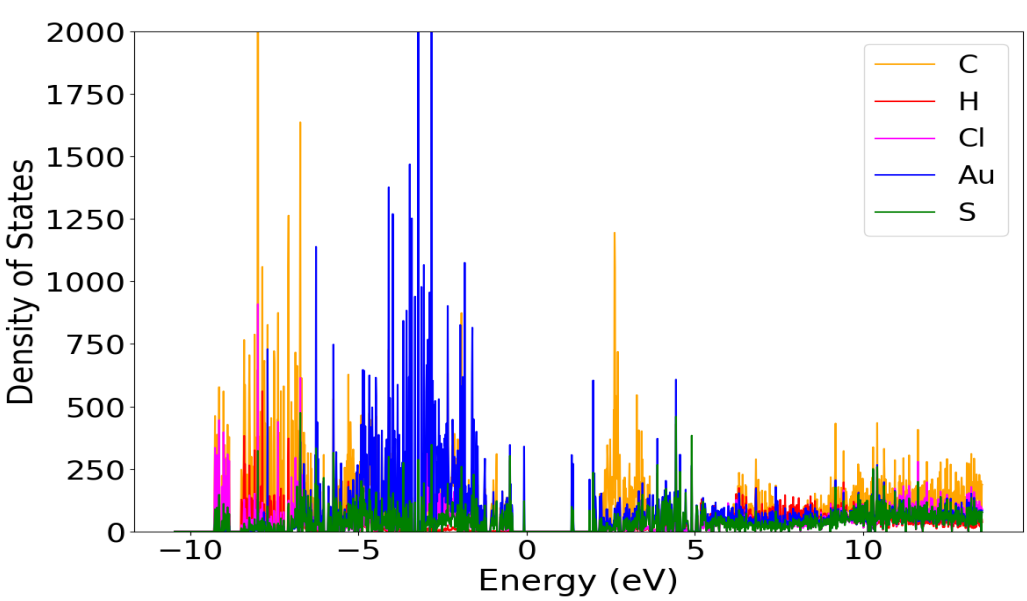
**Table S3.** Electronic properties of the $[Au_{25}(XBT)_{18}]^-$ NCs, X = F, Cl, Br.

| | | | |
|---|---|---|---|
| Lattice vectors | a= 29.899<br>b= 17.874<br>c= 35.269 | a= 29.899<br>b= 17.874<br>c= 35.269 | a= 29.899<br>b= 17.874<br>c= 35.269 |
| Chemical Formula | $Au_{100}S_{72}C_{432}H_{288}F_{72}$ | $Au_{100}S_{72}C_{432}H_{288}Cl_{72}$ | $Au_{100}S_{72}C_{432}H_{288}Br_{72}$ |
| Number of Atoms | 964 | 964 | 964 |
| Total Energy (eV) | -54996566.84262 | -55706315.966422088 | -59941358.851653107 |
| Fermi Energy (eV) | -5.72342 | -5.54215765 | -5.48438 |
| Highest occupied state (eV) | -5.72342 | -5.55704335 | -5.492457 |
| Lowest unoccupied state (eV) | -4.36278 | -4.20388263 | -4.16609 |
| Estimated HOMO-LUMO gap (eV) | 1.37640 | 1.35316072 | 1.32630 |
| Cell Volume ($Å^3$) | 17252.96791 | 17252.96791 | 17252.96791 |

a)


2000
1750
1500
1250
1000
750
500
250
0
Density of States
−10
−5
0
5
10
Energy (eV)
C
H
Au
S
F

b)


2000
1750
1500
1250
1000
750
500
250
0
Density of States
−10
−5
0
5
10
Energy (eV)
C
H
Cl
Au
S

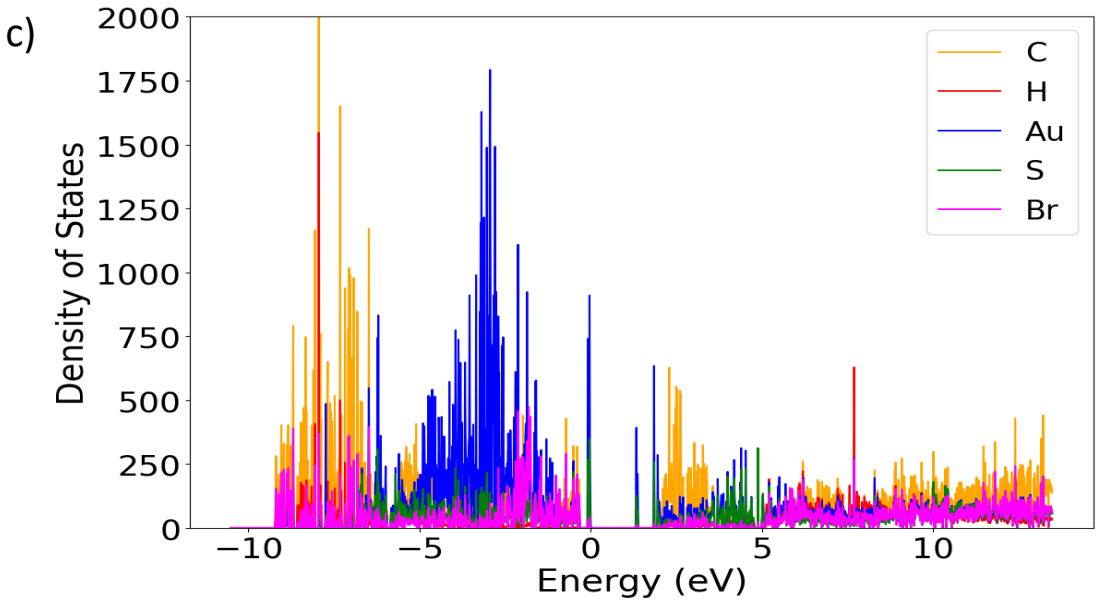



**Figure S7.** Density of states of the a) $[Au_{25}(FBT)_{18}]^-$, b) $[Au_{25}(CBT)_{18}]^-$, c) $[Au_{25}(BBT)_{18}]^-$ NCs.

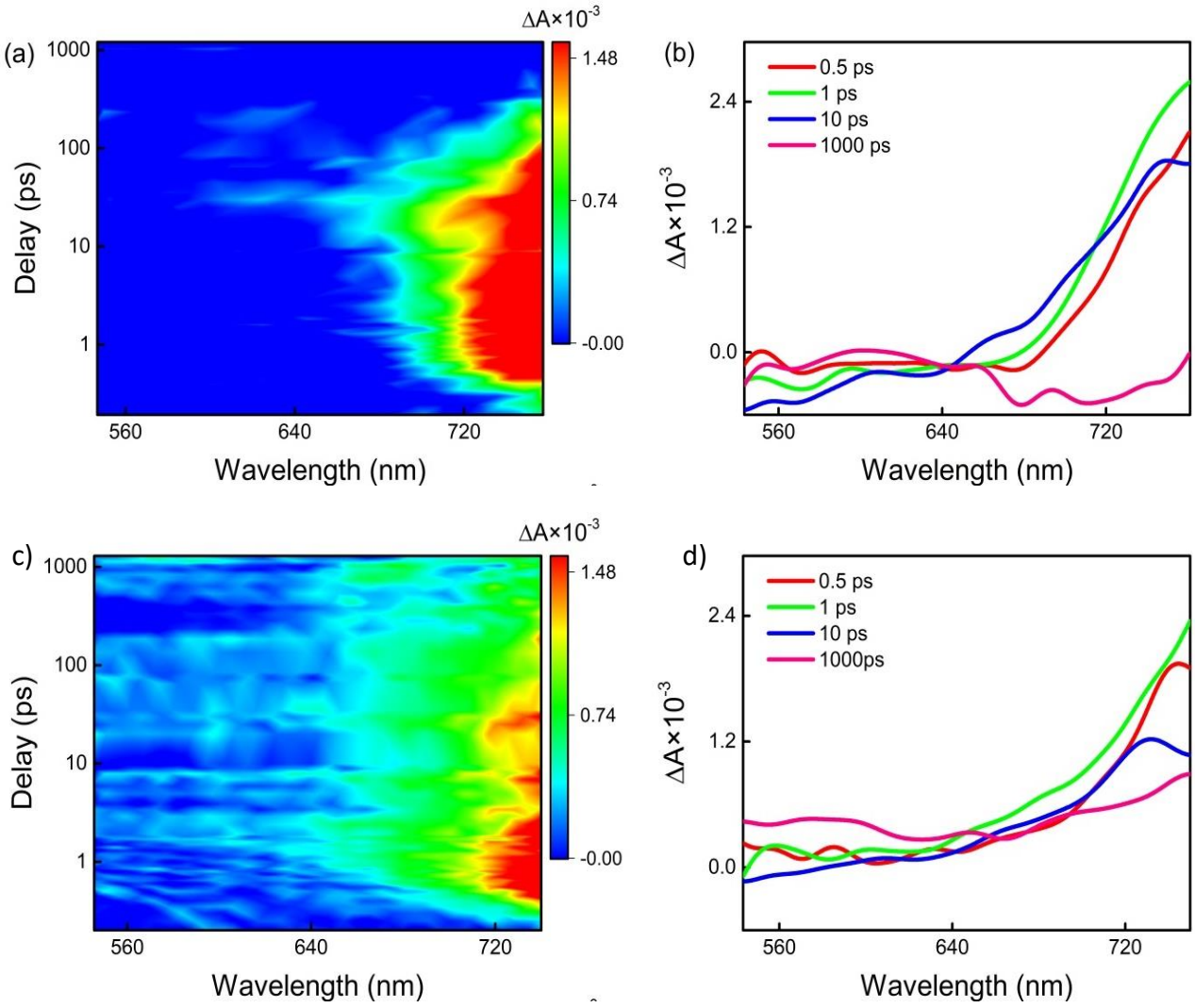



**Figure S8.** Contour plot illustrating the ultrafast transient absorption spectrum of (a) $[Au_{23}(S\text{-}c\text{-}C_6H_{11})_{16}]^-$ NC and (c) $Au_{23}(S\text{-}c\text{-}C_6H_{11})_{17}$ NCs dissolved in dichloromethane (DCM), with (b & d) corresponding cross-sections of the contour plot at selected probe delay times. The excitation wavelength is 400 nm, and the excitation fluence is 490 nJ/cm².

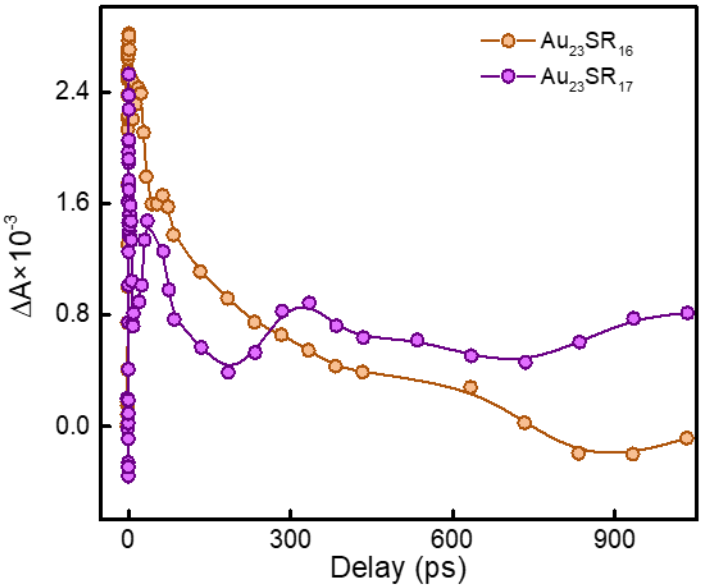
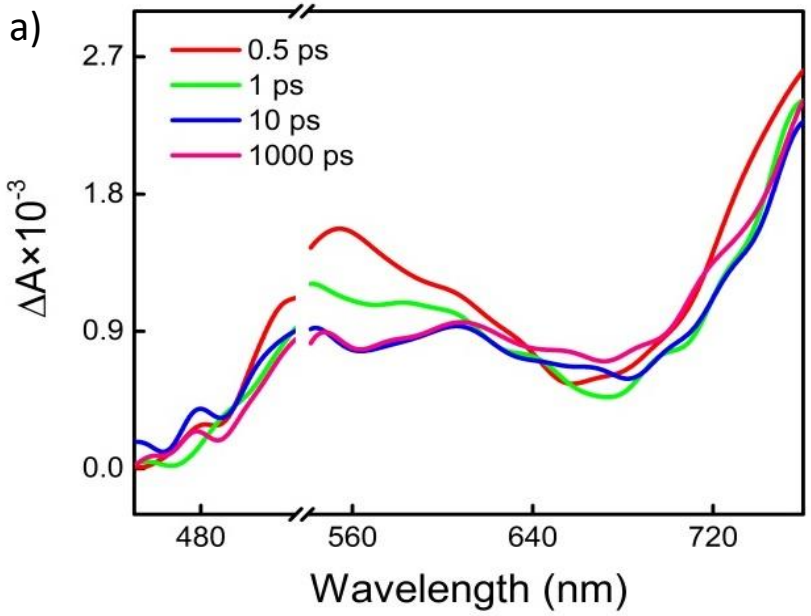



**Figure S9.** TA decay kinetics of the $[Au_{23}(S\text{-}c\text{-}C_6H_{11})_{16}]^-$ and the $Au_{23}(S\text{-}c\text{-}C_6H_{11})_{17}$ species at 750 nm.



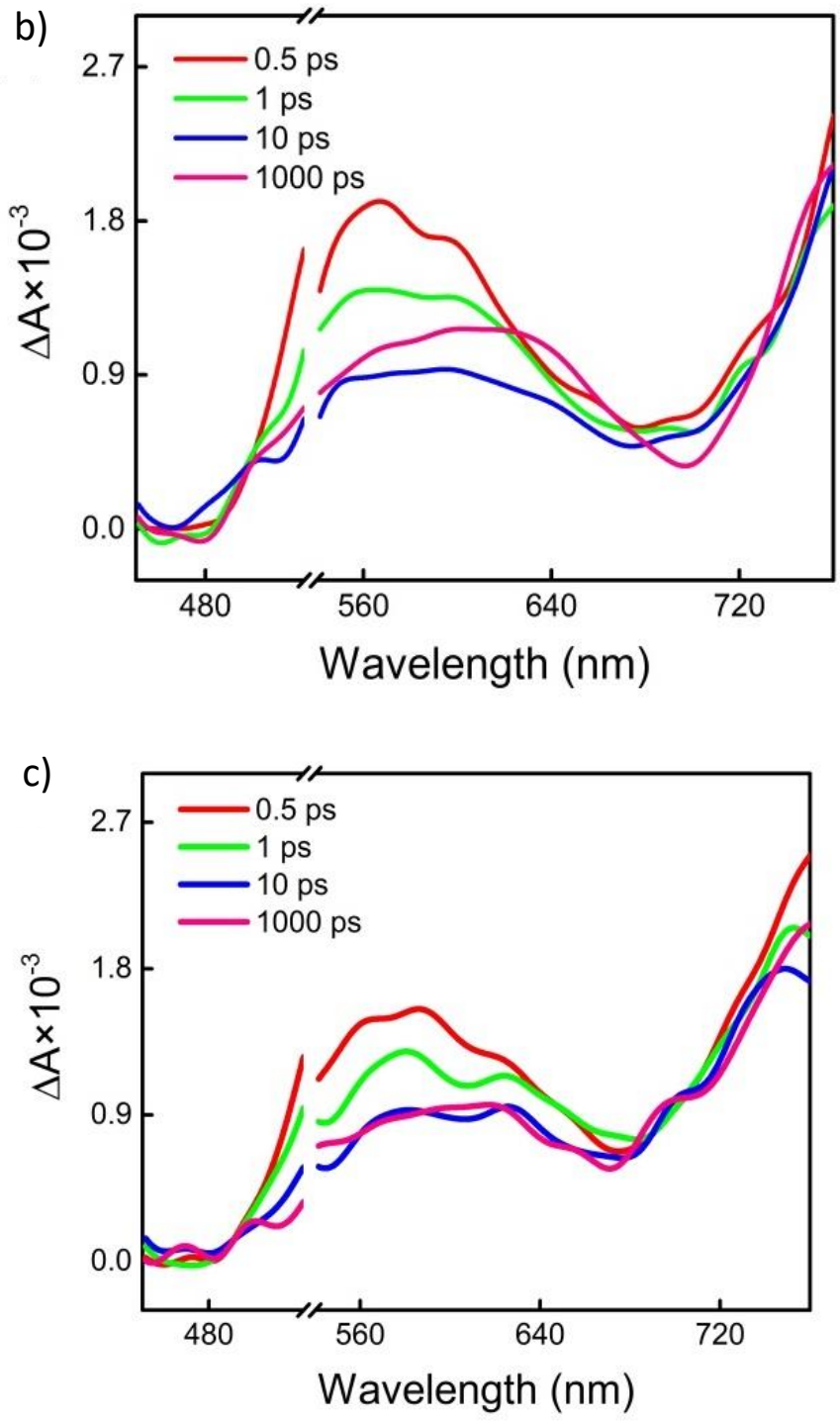



**Figure S10.** The time-associated femtosecond transient absorption spectra of the a) $[Au_{25}(FBT)_{18}]^-$, b) $[Au_{25}(CBT)_{18}]^-$, c) $[Au_{25}(BBT)_{18}]^-$ NCs at different delay times.

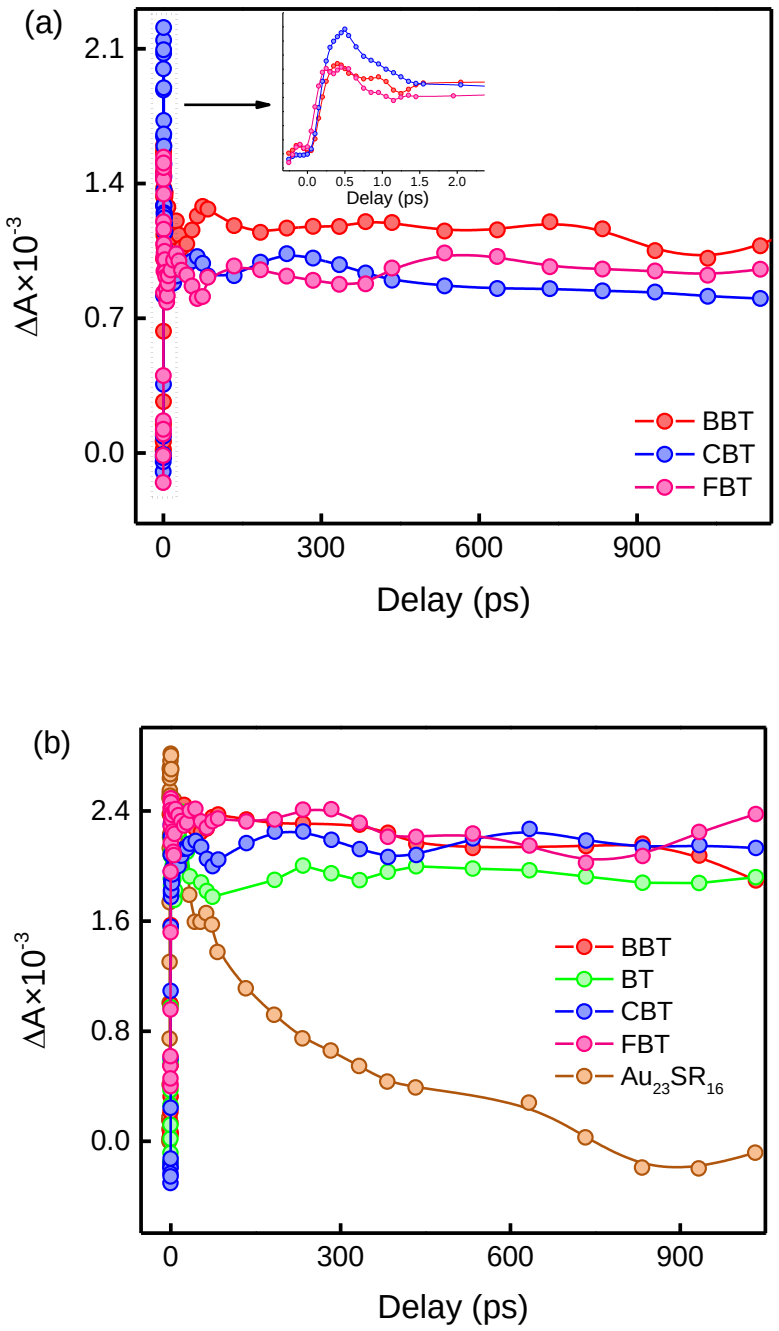



**Figure S11**. TA decay kinetics of the $[Au_{25}(XBT)_{18}]^-$ NCs at (a) 560 nm. TA decay kinetics of the $[Au_{25}(XBT)_{18}]^-$ NCs and the $[Au_{23}(S\text{-}c\text{-}C_6H_{11})_{16}]^-$ at (b) 750 nm. Inset of (a) shows the early time decay feature of PIA.

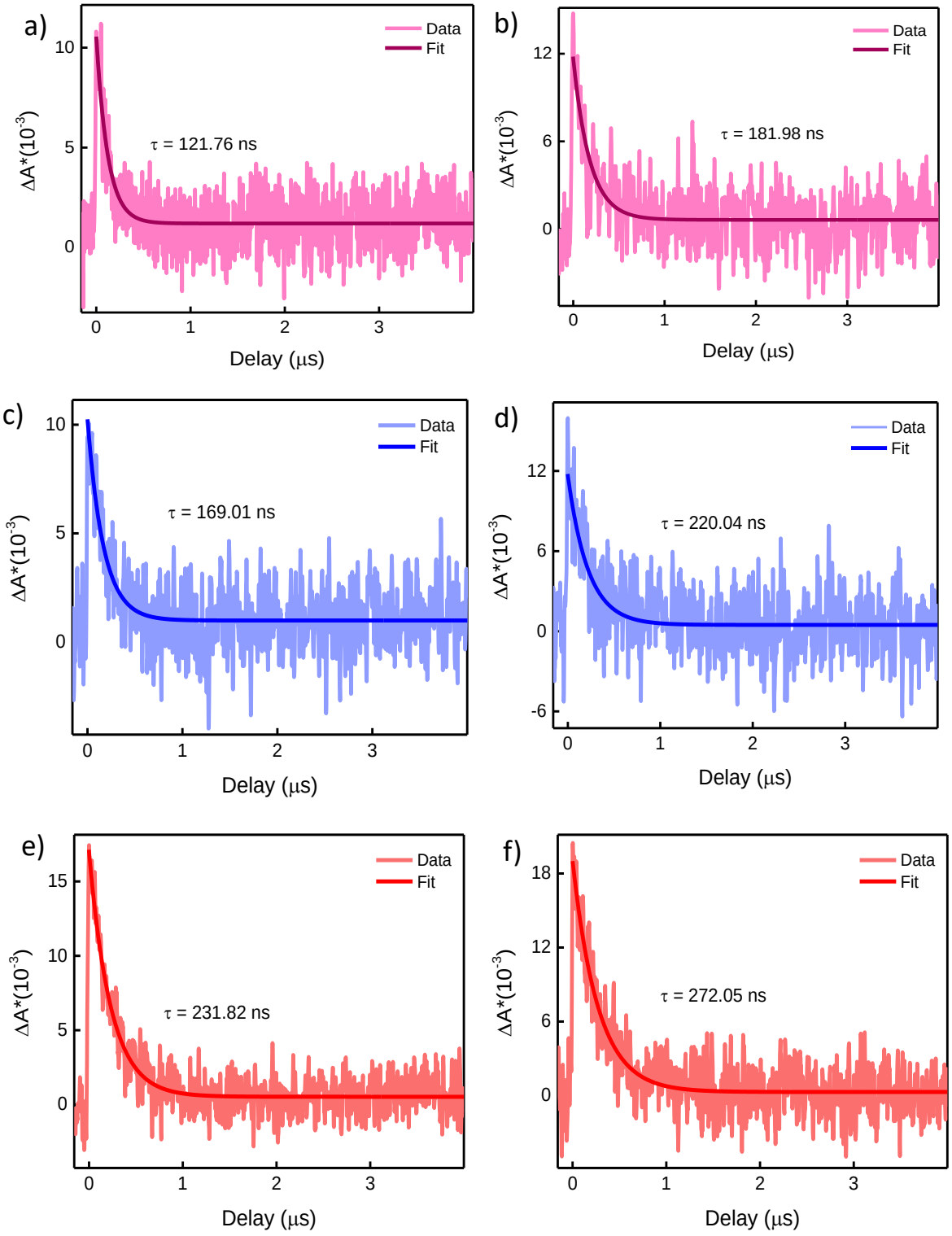



**Figure S12.** Nanosecond transient absorption decay kinetics of a), b) $[Au_{25}(FBT)_{18}]^-$ NC; c), d) $[Au_{25}(CBT)_{18}]^-$ NC; e), f) $[Au_{25}(BBT)_{18}]^-$ NCs at 560 nm and 750 nm wavelength, respectively.

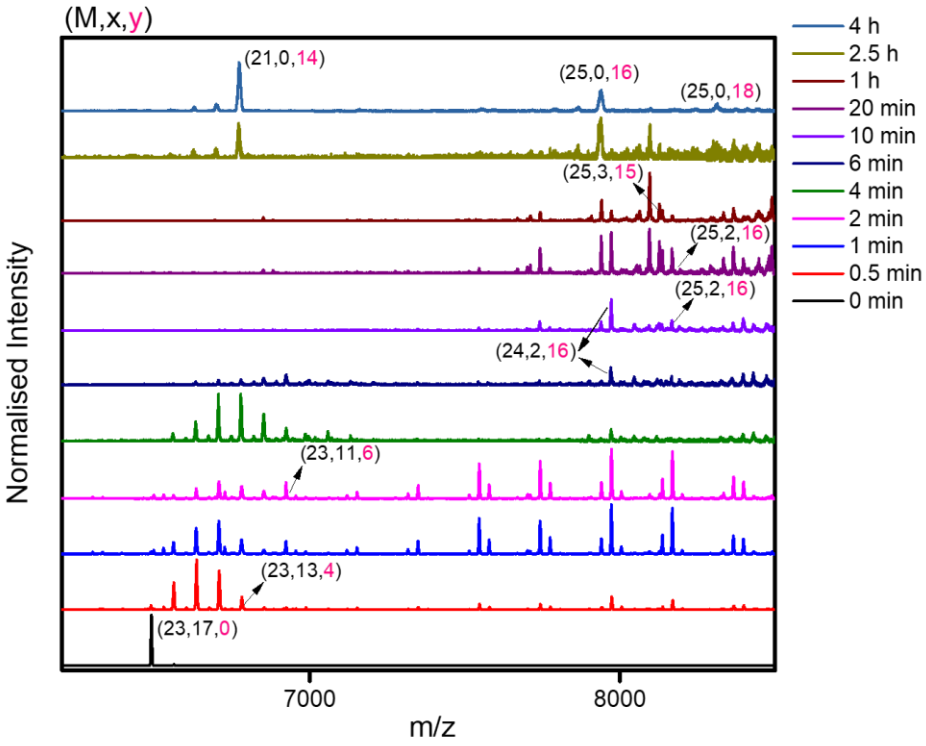



**Figure S13 a.** Time-dependent MALDI-MS spectra of the aliquots taken during the transformation reaction of $Au_{23}(S\text{-}c\text{-}C_6H_{11})_{17}$ intermediate species with BBT. (M = number of metal atoms, x = number of cyclohexanethiolate ligands, y = number of bromobenzenethiolate ligands in each species).

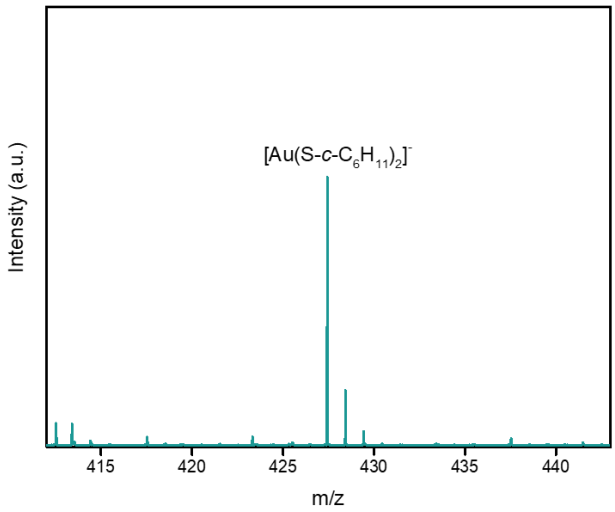



**Figure S13 b.** Negative mode ESI-MS spectrum of the $[Au_{23}(S\text{-}c\text{-}C_6H_{11})_{16}]^-$ nanoclusters at low range showing the presence of $Au(S\ S\text{-}c\text{-}C_6H_{11})_2$ complex.

**Table S4**. Optimized structure coordinates of a) $[Au_{23}(SC_6H_{11})_{16}]^-$ NC, b) $Au_{23}(SC_6H_{11})_{17}$, c) $Au_{23}(SC_6H_{11})_{11}(BBT)_6$, d) $Au_{24}(SC_6H_{11})_2(BBT)_{16}$, e) $Au_{25}(SC_6H_{11})_2(BBT)_{16}$ and f) $[Au_{25}(BBT)_{18}]^-$ NCs.

**a) $Au_{23}(S\text{-}c\text{-}C_6H_{11})_{16}$**

| | | | |
|---|---|---|---|
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| Au | 14.447284570 | 12.224959686 | 14.863527453 |
| Au | 15.967930274 | 17.601810981 | 14.917166678 |
| Au | 16.504536438 | 13.074043281 | 13.249575970 |
| Au | 13.998098032 | 16.733273335 | 16.597286586 |
| Au | 17.968017113 | 15.684234418 | 16.134212154 |
| Au | 12.362642886 | 14.044246017 | 13.551292102 |
| Au | 12.786353950 | 14.090446579 | 16.318446428 |
| Au | 17.700752324 | 15.729175244 | 13.434698520 |
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| Au | 19.164315297 | 18.296354055 | 14.195912140 |
| Au | 11.107849880 | 11.734659456 | 15.606409317 |
| Au | 21.166843754 | 16.105834297 | 15.894804183 |
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| S | 18.351040772 | 11.598814523 | 17.377324218 |

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**e) $Au_{25}(S\text{-}c\text{-}C_6H_{11})_2BBT_{16}$**

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| Au | 14.904742194 | 15.066300155 | 15.017291948 |
| Au | 14.839122256 | 17.814040133 | 14.274113112 |
| Au | 15.085189745 | 12.267778725 | 15.650537922 |

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| Au | 15.028648242 | 15.540119125 | 12.128844278 |
| Au | 14.823132463 | 14.599976948 | 17.877285506 |
| Au | 16.102003702 | 13.109314199 | 13.208788168 |
| Au | 13.776343932 | 17.114169994 | 16.739634091 |
| Au | 12.627302361 | 16.053470250 | 13.545801509 |
| Au | 17.179910714 | 14.095524537 | 16.464766112 |
| Au | 12.729043710 | 13.823496231 | 16.243742235 |
| Au | 17.153480095 | 16.166738674 | 13.767477795 |
| Au | 16.600583680 | 16.842433007 | 16.597827543 |
| Au | 13.246220450 | 13.330381040 | 13.402359722 |
| Au | 12.125670099 | 19.084625637 | 14.937740103 |
| Au | 17.887080233 | 11.126480624 | 14.871080430 |
| Au | 15.132692698 | 19.994819111 | 16.698782177 |
| Au | 14.857788704 | 10.345448507 | 13.172595204 |
| Au | 10.239446127 | 13.625085086 | 13.993472230 |
| Au | 19.613475759 | 16.386802637 | 16.046928034 |
| Au | 11.917929274 | 14.602863345 | 10.962984838 |
| Au | 17.961403545 | 15.385147033 | 19.072659544 |
| Au | 17.735238616 | 14.999629845 | 10.866936216 |
| Au | 12.209778484 | 15.069158181 | 19.139355521 |
| Au | 16.556099030 | 18.303781654 | 11.414019924 |
| Au | 13.406210831 | 11.766572883 | 18.546364873 |
| S | 9.789160456 | 14.206314947 | 11.800914772 |
| S | 20.082847241 | 15.787790871 | 18.231114980 |
| S | 13.969575206 | 15.129016481 | 10.002231338 |
| S | 15.875118215 | 14.990203514 | 20.016490516 |
| S | 17.656838986 | 12.741204962 | 11.409107663 |
| S | 12.343171583 | 17.335217875 | 18.639302735 |
| S | 10.434849903 | 13.140316576 | 16.250254640 |
| S | 19.431304079 | 16.884538852 | 13.793760334 |

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| S | 13.293807968 | 20.937561137 | 15.657562723 |
| S | 17.025666601 | 9.547228782 | 13.403194850 |
| S | 10.826621937 | 17.588067696 | 13.725099692 |
| S | 18.997122223 | 12.547199774 | 16.332917542 |
| S | 18.113612129 | 17.172440512 | 10.144711993 |
| S | 11.777293739 | 12.866780779 | 19.755175157 |
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| S | 15.165021798 | 19.638062418 | 12.699886095 |
| S | 14.862113037 | 10.484029271 | 17.272495349 |
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| Br | 22.664212166 | 12.333470511 | 10.515779954 |
| Br | 13.283463579 | 20.691909057 | 6.779494409 |
| Br | 16.216215679 | 9.633486482 | 23.625488436 |
| Br | 18.882895893 | 19.526497832 | 23.438032150 |
| Br | 11.126362022 | 10.292455935 | 6.624745275 |
| Br | 19.915406980 | 9.223470129 | 21.810022828 |
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| C | 20.872066575 | 17.158617297 | 20.481823188 |
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| C | 12.548444506 | 12.435179923 | 24.237314190 |
| C | 7.777746815 | 10.782863881 | 9.554624262 |
| C | 22.135700355 | 19.207477940 | 20.447799944 |
| C | 16.848329761 | 10.558537403 | 9.962689038 |
| C | 13.754234337 | 19.354358055 | 19.871991600 |
| C | 13.710347542 | 16.677668229 | 9.162914315 |
| C | 16.023994089 | 13.486547192 | 20.959757337 |
| C | 13.711635208 | 16.668492035 | 7.761073638 |
| C | 15.884150814 | 13.586306184 | 22.351710383 |

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| C | 18.461654157 | 20.224585089 | 19.353511121 |
| C | 11.368782070 | 9.885471048 | 10.762001150 |
| C | 15.890393551 | 10.633271398 | 7.752817234 |
| C | 14.232433103 | 19.439827564 | 22.228543024 |
| C | 15.946881867 | 5.763074031 | 14.376158504 |
| C | 19.137291295 | 11.636125319 | 17.858608524 |
| C | 16.352354118 | 9.892879788 | 8.842857743 |
| C | 14.258937715 | 20.045015182 | 20.971085534 |
| C | 17.407320129 | 16.256010899 | 6.237909069 |
| C | 12.052532564 | 13.641943205 | 23.740849388 |
| C | 15.908296624 | 12.028793342 | 7.778443373 |
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| C | 16.245847043 | 12.235118029 | 20.371931430 |
| C | 18.507147190 | 10.400859938 | 18.071433534 |
| C | 19.988878747 | 12.151870257 | 18.848216601 |
| C | 17.359097690 | 18.484704025 | 21.250063658 |
| C | 12.644747203 | 11.396201449 | 8.784474947 |
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| C | 13.781084674 | 9.228110810 | 16.608756589 |
| C | 18.839975473 | 20.331421035 | 20.692353198 |
| C | 11.022764458 | 9.701205219 | 9.422835963 |
| C | 16.013839371 | 7.019620744 | 13.778559101 |

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| C | 8.766852323 | 14.143277989 | 18.181537798 |
| C | 21.138268054 | 15.972057026 | 11.858741751 |
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| C | 18.749676376 | 9.674060767 | 19.236419504 |
| C | 20.216796720 | 11.441056389 | 20.025809603 |
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| C | 16.168257033 | 11.206221629 | 22.548492135 |
| C | 17.684098905 | 6.421707723 | 15.943660877 |
| C | 16.775437385 | 5.477235136 | 15.463442194 |
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| C | 12.178679255 | 7.195887214 | 15.583354375 |
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| C | 18.366803629 | 21.324666491 | 14.604353337 |
| C | 11.779934748 | 8.525982847 | 15.432466483 |
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| C | 12.902947159 | 23.238659934 | 17.141814624 |
| C | 11.921970823 | 24.210211759 | 17.815279633 |
| C | 11.157992036 | 23.534537990 | 18.959822054 |
| C | 10.446973897 | 22.261890178 | 18.483521320 |
| C | 11.426554698 | 21.290137746 | 17.808522338 |
| C | 10.618703885 | 18.600166771 | 12.172524698 |
| C | 9.724810527 | 19.804741237 | 12.494122416 |
| C | 9.473905677 | 20.647662814 | 11.236016656 |
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| H | 11.621740430 | 18.954443426 | 11.890005116 |
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| H | 11.420117438 | 22.284826705 | 15.902265742 |
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| H | 12.465172294 | 25.095982802 | 18.178434349 |
| H | 11.202122028 | 24.573931422 | 17.060703317 |

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| H | 10.430594499 | 24.236173255 | 19.395961627 |
| H | 11.867102205 | 23.275603900 | 19.765994717 |
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| H | 9.650777255 | 22.532894356 | 17.767892130 |
| H | 10.905904147 | 20.395438978 | 17.434527413 |
| H | 12.158566431 | 20.943342520 | 18.552018459 |
| H | 16.388069958 | 13.777277422 | 8.935997028 |
| H | 12.851003953 | 16.447447792 | 21.398233098 |
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| H | 11.436964416 | 14.711540541 | 21.974085536 |
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| H | 13.216263821 | 10.429003483 | 23.782592062 |
| H | 8.435213043 | 11.786663799 | 7.755548916 |
| H | 21.579951591 | 18.161326001 | 22.257170023 |
| H | 8.431238770 | 11.786180732 | 12.735996786 |
| H | 21.341919007 | 18.252650701 | 17.283658094 |
| H | 7.271073158 | 9.969287838 | 11.493134329 |
| H | 22.530532462 | 20.066241053 | 18.502964711 |
| H | 17.232456301 | 9.978695665 | 10.801298028 |
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| H | 10.861433673 | 9.307469329 | 11.535355821 |
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| H | 16.334375429 | 8.803897032 | 8.816315933 |

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| H | 13.755586070 | 17.661621559 | 23.362790114 |
| H | 16.205569735 | 17.685846672 | 19.616281816 |
| H | 13.804347655 | 12.244657431 | 10.390167801 |
| H | 13.587232782 | 17.853334318 | 5.958366479 |
| H | 15.850606251 | 12.524945552 | 24.234771932 |
| H | 13.539198576 | 17.890501512 | 10.938641506 |
| H | 16.385410883 | 12.157684978 | 19.293578347 |
| H | 17.814706110 | 10.007751158 | 17.326323845 |
| H | 20.485640272 | 13.110106391 | 18.694613672 |
| H | 16.929908045 | 17.805176460 | 21.985124974 |
| H | 13.135629830 | 11.987845662 | 8.014405451 |
| H | 19.572606605 | 21.076907030 | 20.999238001 |
| H | 10.251607387 | 8.983103237 | 9.146692059 |
| H | 15.347157246 | 7.258588601 | 12.948748529 |
| H | 8.666854413 | 13.104474037 | 18.497649085 |
| H | 21.192411453 | 17.017467157 | 11.553784549 |
| H | 10.321281469 | 16.061008163 | 15.829257495 |
| H | 19.666632699 | 13.965786479 | 14.188282416 |
| H | 7.514825755 | 14.903959126 | 19.770932220 |
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| H | 18.467852328 | 8.415133770 | 15.695992520 |
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| H | 20.901709765 | 12.234398781 | 12.917266823 |
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| H | 18.266006859 | 8.709160049 | 19.390023324 |

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| H | 18.333969515 | 6.186105980 | 16.786218631 |
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| H | 13.656366166 | 5.825227151 | 16.368474217 |
| H | 17.875464590 | 19.368842557 | 13.852957616 |
| H | 12.285512175 | 10.581660527 | 15.832603312 |
| H | 14.898785340 | 22.426476615 | 13.229866503 |
| H | 15.092687607 | 7.638068757 | 17.269244166 |
| H | 19.331111538 | 21.012029778 | 15.002609313 |
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**f) $Au_{25}BBT_{18}$**

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| Au | 14.920378185 | 17.770701426 | 14.342956709 |
| Au | 15.079262062 | 12.227295274 | 15.656394880 |
| Au | 15.097394636 | 15.518376356 | 12.101143874 |
| Au | 14.903269826 | 14.480722702 | 17.899181587 |
| Au | 16.108061099 | 13.040250000 | 13.191981072 |
| Au | 13.892054501 | 16.956165568 | 16.806499532 |
| Au | 12.746620756 | 15.998558289 | 13.568257121 |
| Au | 17.254336060 | 13.999336665 | 16.432333383 |
| Au | 12.759872524 | 13.924584348 | 16.267862866 |
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| Au | 16.728903884 | 16.735303624 | 16.553982798 |
| Au | 13.271875213 | 13.263516636 | 13.445273242 |
| Au | 12.081046389 | 18.959743815 | 15.132393203 |
| Au | 17.917743072 | 11.032506127 | 14.873277651 |
| Au | 15.153349076 | 19.729970538 | 16.805076328 |
| Au | 14.846765398 | 10.264853592 | 13.196442999 |
| Au | 10.290552641 | 13.705407119 | 13.991766427 |

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| Au | 19.711630911 | 16.294624419 | 16.008049869 |
| Au | 11.918336199 | 14.712765580 | 10.949080045 |
| Au | 18.082788082 | 15.288081118 | 19.051686784 |
| Au | 17.784439331 | 14.921920245 | 10.889991797 |
| Au | 12.213135254 | 15.074289716 | 19.109496447 |
| Au | 16.595544956 | 18.240061395 | 11.452791287 |
| Au | 13.403262944 | 11.756289539 | 18.548856550 |
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| S | 20.193158008 | 15.706687599 | 18.192124062 |
| S | 13.988977460 | 15.133354889 | 9.998108959 |
| S | 16.012074637 | 14.865908083 | 20.001881497 |
| S | 17.672637413 | 12.657138268 | 11.410017892 |
| S | 12.323139346 | 17.337306470 | 18.585083526 |
| S | 10.483671224 | 13.200872455 | 16.242531028 |
| S | 19.518117099 | 16.796959447 | 13.756723113 |
| S | 12.982426705 | 20.524910320 | 16.589097923 |
| S | 17.016571610 | 9.467517050 | 13.416180468 |
| S | 10.941343690 | 17.555982410 | 13.676940591 |
| S | 19.057677725 | 12.439584196 | 16.325535560 |
| S | 18.189420413 | 17.110128126 | 10.223275020 |
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| S | 15.168982894 | 19.553698163 | 12.737255471 |
| S | 14.827073344 | 10.443614900 | 17.261156267 |
| Br | 15.068197463 | 9.683976545 | 6.276810333 |
| Br | 14.928017391 | 20.311444260 | 23.714840651 |
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