# Supporting Information

## $Au_{133}(SPh\text{-}tBu)_{52}$ Nanomolecules: X-ray Crystallography, Optical, Electrochemical and Theoretical Analysis

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## 1. Materials and Instrumentation

**Materials:** 4-*tert*-butylbenzenethiol (TCI, >97%), hydrogen tetrachloroaurate(III) trihydrate (Alfa Aesar, 99.99%), tetra-n-octylammoniumbromide (Acros Organics, 98%), sodium borohydride (Fisher), trans-2-[3[(4-tertbutylphenyl)-2-methyl-2-propenylidene]malononitrile (DCTB matrix) (Fluka ≥ 99%), ethylacetate HPLC grade (Acros Organics), toluene (Fisher), methanol (Fisher), and tetrahyrofuran (Fisher) were purchased and used as received.

**Instrumentation:**

MALDI: Matrix-assisted laser desorption ionization time of fight (MALDI-TOF) mass spectra were collected on a Voyager DE Pro mass spectrometer in linear positive mode using 20 mM DCTB(*14*) as matrix spotted from a THF solution. The broadness of the MALDI peaks in Figure 2a (compared to the ESI peaks) is due in part to the limited instrumental resolution and laser induced fragmentation.

ESI-MS spectra were acquired on Waters Synapt HDMS instrument by dissolving the title compound in HPLC grade THF. $Au_{144}(SCH_2CH_2Ph)_{60}$ was used for calibration checks for ESI. For cesium acetate (CsOAc) experiments, 50mM of cesium acetate dissolved in dry ethanol was added into a THF solution of the nanomolecules in 3:50 v/v CsOAc:nanomolecule ratio.

Electrochemical measurements were performed on a CHI 620 instrument in anhydrous 1,2-dichloroethane solution with 0.5 mM bis(triphenyl phosphoranylidene) ammonium tetrakis (pentafluorophenyl) borate [$BTPPATBF_{20}$] as supporting electrolyte under nitrogen atmosphere. A three electrode setup with platinum working electrode, platinum wire counter electrode and Ag/AgCl reference electrode were used. DPV measurements were performed at a scan rate of 4 mV/s, pulse height of 0.05 V, pulse width of 0.2 s and pulse period of 0.05 s.

UV-visible absorption spectra were recorded in Me-THF solution on a Cary 5000 spectrophotometer equipped with a Janis VNF-100 liquid nitrogen optical cryostat for low temperature measurements. In Figure 3(a) the optical spectra at two different temperatures: 88 and 258 K are reported, to underline the different response of the bands at [2.49–2.91] eV and [3.59–3.81] eV to thermal effects.

TEM samples were prepared by drop casting a toluene solution of nanoparticles suspension onto lacey carbon films supported on Cu grids. Images were acquired in a JEOL 2100 using 200 kV.

The SAXS data collections were performed at the 12ID-B beam line of Advance Photon Source (APS) located in Argonne national laboratory using 12keV X-ray energy. The SAXS data were collected with Pilatus 2M detector (DECTRIS Ltd.) cut-off energy was set as 10 keV to eliminate possible fluorescence background. Exposure times of 1s were used for the measurements. The data was reduced to intensity vs scattering vector ($q$) profiles, and background subtracted, using the software package at the beamline. The pair distance distribution function, p(r), derived from SAXS data was obtained using the program GNOM,(*26*) fitting scattering data up to 0.8 $Å^{-1}$. The SAXS data was collected on a statistically significant population of ca. $10^{11}$ particles.

NMR spectroscopy of the title compound was attempted, but did not yield meaningful data. Due to the non-trivial nature of the NMR study of large (>100 Au atoms) nanoparticles, a further detailed study will be conducted in the future and is beyond the scope of this study. TGA was not conducted due to limited sample availability and the destructive nature of the technique.

A suite of techniques used for the title compound include: (conclusive results) X-ray crystallography, high-resolution ESI mass spectrometry and theoretical analysis; (supporting results) MALDI mass spectrometry, small angle X-ray scattering, and TEM.

## 2. Experimental methods

a. Synthesis

The synthesis and isolation of $Au_{133}(SPh\text{-}tBu)_{52}$ was performed in three steps. This three step procedure is described elsewhere in detail.(*27,28*) First, a polydisperse crude mixture was synthesized in a single phase reaction by modifying a reported process. Second, the crude mixture was subjected to thermochemical treatment with excess thiol under specific conditions. Finally, size exclusion chromatography(*29*) technique was used to isolate pure monodisperse nanomolecules.

Step 1: $HAuCl_4.3H_2O$ (0.3g) and TOABr (0.42g, Au:TOABr = 1:1) were dissolved in ethyl acetate(*30*) (30 mL) in a 100 mL round-bottom flask and stirred for 2 hours at 500 rpm. Thereafter, 4-tertbutylbenzenethiol (Au: HSPh-*t*Bu = 1:2 mole ratio) was added and stirred for another 4 hours. To this reaction mixture $NaBH_4$ (0.29g, Au:$NaBH_4$ = 1:10) was added rapidly, which turned the solution color to black with the evolution of gas bubbles. After about 24 hours of stirring, the resultant product was dried using rotary evaporation to remove excess solvent. Then, to the crude product a few drops of distilled water was added and washed with methanol 3-4x times to remove excess thiol and other reaction byproducts.

Step 2: The crude mixture was dissolved in a minimum amount of toluene (400µL) and 0.5 mL of 4-tertbutylbenzenethiol in a 10 mL round-bottom flask and subjected to thermochemical treatment or etching(*31*) at 80˚C and stirred for about 6 days at 500 rpm.

Step 3: $Au_{133}(SPh\text{-}tBu)_{52}$ was separated using a 24 inch size exclusion chromatography column packed with Biorad SX1 beads soaked in THF.(*29*) 10-20mg of the etched product was dissolved in minimum amount of stabilized THF (<400µL) and loaded carefully on the flat bed of the column to ensure effective separation. The last few fractions contained $Au_{133}(SPh\text{-}tBu)_{52}$.

b. Crystallization and structure solution

The crystallization was performed using vapor diffusion method. The product was dissolved in 500 µL of dichloromethane in the inner vial and ethanol was used as the non-solvent in the outer vial. Repeated crystallization trials were performed over a period of many months. Crystals were observed in the certain vials after 3-5 days.

A crystal was selected and attached to the tip of a MiTeGen MicroMount. The crystal was mounted in a stream of cold nitrogen at 100(1) K and centered in the X-ray beam using a video camera. The crystal evaluation and data collection were performed on a Bruker APEX II diffractometer with Mo Kα (λ = 0.71073 Å) radiation. The reflections were successfully indexed by using the indexing routine in APEXII program suite. Data were corrected for absorption effects with SADABS using the multiscan technique. The average residual for symmetry equivalent reflections is Rint = 21.89% and Rσ = 9.65%. XPREP determined the space group to be C2/c, with Z = 4 for the formula unit, $C_{520}H_{676}Au_{133}S_{52}$. The structure was solved with XT and subsequent structure refinements were performed with XL(*32*) using Olex2 program.(*33*) The

final anisotropic full-matrix least-squares refinement on Fo2 with 837 variables converged at R1 = 8.41% for the observed data and wR2 = 28.29% for all data. The goodness-of-fit was 1.327. The largest peak on the final difference electron density synthesis was 2.62 e-/Å3 and the deepest hole was -1.90 e-/Å3 with an RMS deviation of 0.33 e-/Å3. On the basis of the final model, the calculated density is 3.016 g/cm3 and F(000) = 60524. CCDC number is 993929.

Due to the large number of very heavy atoms, the refinement required some handling beyond that of a typical structure determination. The asymmetric unit is ½ molecule, second half is generated by 2-fold rotation. The Au atoms were freely refined with full anisotropic parameters for thermal motion. Sulfur atoms were similarly handled, and three required mild isotropic restraints. All Au and S atoms were readily located during structure solution and initial refinement. Carbon atoms were located through successive cycles of least-squares refinement followed by difference Fourier synthesis. On locating 3 atoms of a phenyl ring, the set was calculated as a complete phenyl ring and constrained to a regular hexagon with the commands available in SHELXL-2014. All but one ring of the asymmetric unit were found and successfully modeled in this fashion. Carbon atoms were refined with isotropic thermal parameters. Two complete t-Butyl groups were found in the asymmetric unit by difference map. It was not possible to locate all of the Me atoms of the remaining *t*Bu groups. Restraints were applied with SADI to maintain interatomic contacts. All C atoms were restrained with SIMU. Due to the weak data and the influence of the many Au atoms, no H atoms were modeled. Hydrogen atoms and all carbon atoms for the proposed structure were included in the chemical formula and dependent calculations for density and F(000).

### 3. Theoretical Methods

**Structure prediction:** Local geometry relaxations and Ab Initio Molecular Dynamics (AIMD) runs were performed using the CP2K code(*34*) whose DFT algorithms are based on a hybrid Gaussian/Plane-Wave scheme (GPW).(*35*) The Perdew–Burke–Ernzerhof (PBE) exchange-correlation (xc-) functional(*19*) was employed in all the total energy simulations. We chose pseudopotentials derived by Goedecker, Teter and Hutter to describe the core electrons of all atoms(*36*) and DZVP basis sets(*37*) to represent the DFT Kohn–Sham orbitals. The cut-off for the auxiliary plane wave representation of the density was 300 Ry. AIMD runs used a time step of 1.0 fs and the temperature was controlled by Nosé–Hoover chain thermostats.(*38*) The $Au_{133}$ core was kept frozen during the AIMD simulations, assuming that the positions of these heavy atoms were correctly determined by X-ray measurements. AIMD simulations and final local relaxation were conducted sequentially, with each starting from starting from the output of the previous simulation (a time average in the case that this was an AIMD run). It can be noted that the rhombicosidodecahedral shell of 60 atoms grows in anti-Mackay stacking with respect to the icosahedral $Au_{55}$ core, but this stacking is not kept for the 12 Au atoms merging into 4 to give the 52-atom hybrid outer Au shell as described in the main text, and moreover in the final minor rearrangement of the Au52 shell of $Au_{133}(SPh\text{-}tBu)_{52}$ – see Fig. 1g-h – one observes a partial shift from anti-Mackay hollow to bridge epitaxy with respect to the underlying icosahedral core.

**Optical prediction:** The optical spectra were simulated performing TDDFT calculations using a real-space approach and the Local Density Approximation (LDA) exchange-correlation functional with the CP2K code. The Local Density Approximation (LDA) exchange-correlation functional was used in TDDFT calculations (in the simulation of the optical response) rather than the PBE one to reduce the computational effort. Starting from a ground-state calculation, optical response is

obtained by subjecting the system to electrical pulses (with a strength 0.001 a.u) in each of the three Cartesian directions and using the time-evolution formalism(*39*) to follow the electron dynamics. A total of 9 femtosec were sampled using a time step of 0.012 femtosec. A time damping of 7.2 femtosec (corresponding to a full width at half maximum of 0.25 eV) was chosen to broaden the predicted spectrum. Molecular boundary conditions were obtained by solving the Poisson equation with a wavelet basis set, see Ref.[10] for more details.

**4. Crystallographic structure** (Image below shows the structure in Figure 1 of the main manuscript, with incomplete ligands. 50 phenyl rings and 8 t-butyl groups were identified)

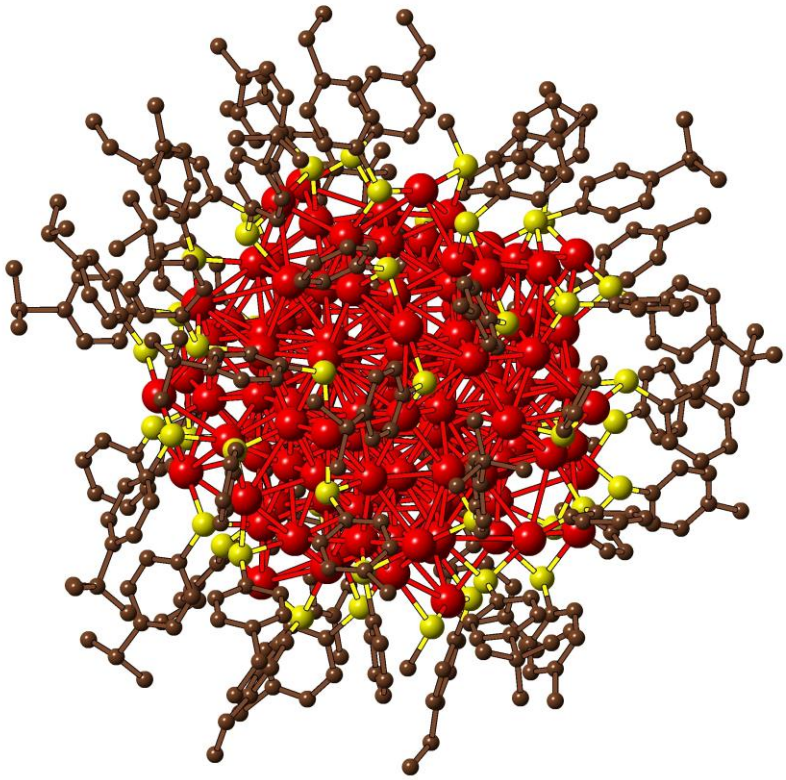

**Table S1. Crystal data and structure refinement for Au133S52**

| | |
|---|---|
| Identification code | mu |
| Empirical formula | $C_{520}H_{672}Au_{133}S_{52}$ |
| Formula weight | 34786.20 |
| Temperature/K | 100(2) |
| Crystal system | monoclinic |
| Space group | C2/c |
| a/Å | 48.626(6) |
| b/Å | 38.971(5) |
| c/Å | 40.431(5) |
| α/° | 90 |

| | |
|---|---|
| β/° | 90.252(4) |
| γ/° | 90 |
| Volume/Å$^3$ | 76614(16) |
| Z | 4 |
| $\rho_{calc}$mg/mm$^3$ | 3.016 |
| μ/mm$^{-1}$ | 25.523 |
| F(000) | 60524 |
| Crystal size/mm$^3$ | 0.1 × 0.1 × 0.05 |
| 2Θ range for data collection | 1.952 to 37.89° |
| Index ranges | -44 ≤ h ≤ 44, -35 ≤ k ≤ 35, -36 ≤ l ≤ 36 |
| Reflections collected | 343986 |
| Independent reflections | 30138[R(int) = 0.2189] |
| Data/restraints/parameters | 30138/921/1337 |
| Goodness-of-fit on F$^2$ | 1.327 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0841, w$R_2$ = 0.2270 |
| Final R indexes [all data] | $R_1$ = 1591, w$R_2$ = 2829 |
| Largest diff. peak/hole / e Å$^{-3}$ | 2.623/-1.896 |

## 5. Transmission electron microscopy (TEM)

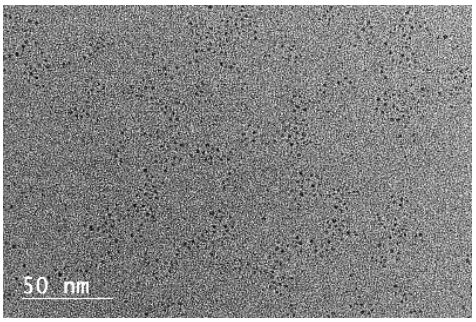


**Figure S1**. TEM image of $Au_{133}(SPh\text{-}tBu)_{52}$ nanomolecules

### 6. Electrospray ionization mass spectrometry of $Au_{133}(SPh\text{-}tBu)_{52}$

Cesium acetate, CsOAc was intentionally added to determine the charge state (fig. S2). CsOAc addition to $Au_{133}(SPh\text{-}tBu)_{52}$, results in the formation of adducts with cesium ions. The major adduct was $[Au_{133}(SPh\text{-}tBu)_{52} \bullet 2Cs^{+}]^{3+}$ which has a nanomolecule charge state of +1. Minor peaks that are less than 10% in peak height include $[Au_{133}(SPh\text{-}tBu)_{52} \bullet 3Cs^{+}]^{3+}$, $[Au_{133}(SPh\text{-}tBu)_{52} \bullet Cs^{+}]^{3+}$ corresponding to charge states of 0, and +2 respectively. This ESI data indicate that the +1 is the preferred charge state, which is in good agreement with the theoretical prediction of a relatively low ionization potential (see below).

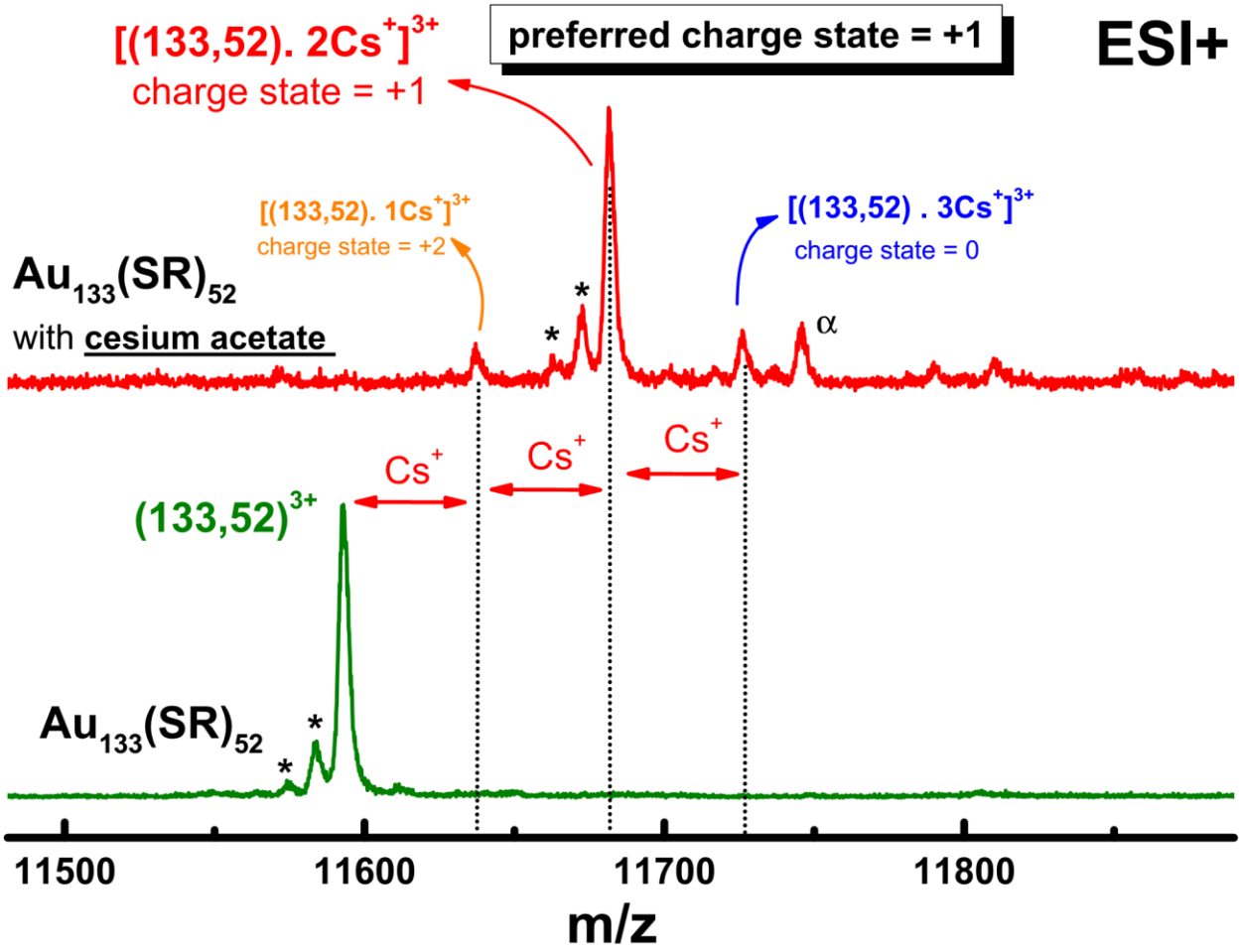


**Figure S2. Preferred charge state is +1**. ESI-MS spectra of the title nanomolecule was acquired after addition of cesium acetate in positive ionization mode. The bottom green plot is the mass spectrum of $Au_{133}(SPh\text{-}tBu)_{52}$ without any salt addition. The top red plot is the mass spectrum of $Au_{133}(SPh\text{-}tBu)_{52}$ with the addition of cesium acetate.(*40*) The peaks indicated by asterisk indicates impurities or other species present in both the spectra. The peak indicated by α could be due to the adduct, $[Au_{133}(SPh\text{-}tBu)_{52} \bullet 2Cs^{+}\ (CsOAc)_1]^{3+}$, which also results in a 1+ charge state. It is well known from literature that ESI-MS routinely yields multiply charged species as opposed to the predominantly singly charged ions in MALDI-MS.(*40,41*) (*27,28,42,43*)

**7. MALDI-MS in the 2,000 to 200,000 m/z range to show purity**

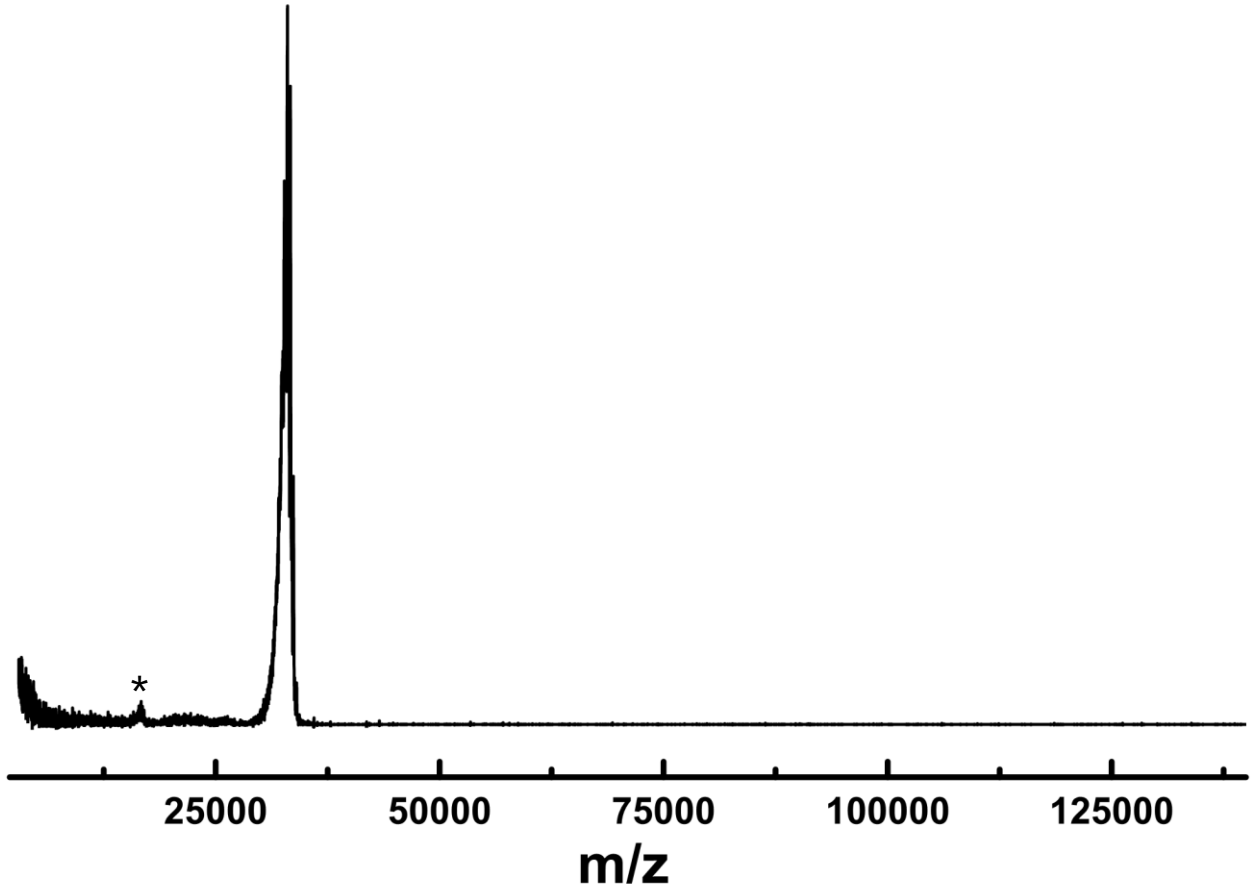


**Figure S3. MALDI-MS in extended mass range to demonstrate purity.** Positive mode MALDI MS data of $Au_{133}(SPh\text{-}tBu)_{52}$ obtained using DCTB matrix.(*14*) The mass spectra was acquired in the 2,000 to 150,000 m/z mass range to show the purity of the $Au_{133}(SPh\text{-}tBu)_{52}$ nanomolecules. The main peak ~33,000 m/z corresponds to the singly charged molecular ion. The minor feature, indicated by the asterisk, ~16,000 m/z corresponds to the double charge molecular ion. The absence of peaks beyond the ~33,000 m/z signal indicate the absence of MALDI signal resulting from larger (>133 Au atom) nanoparticles. It has been reported in multiple reports before that MALDI primarily yields singly charged species.(*27,28,42,43*)

**8. MALDI-MS using high laser fluence (to probe the purity)**

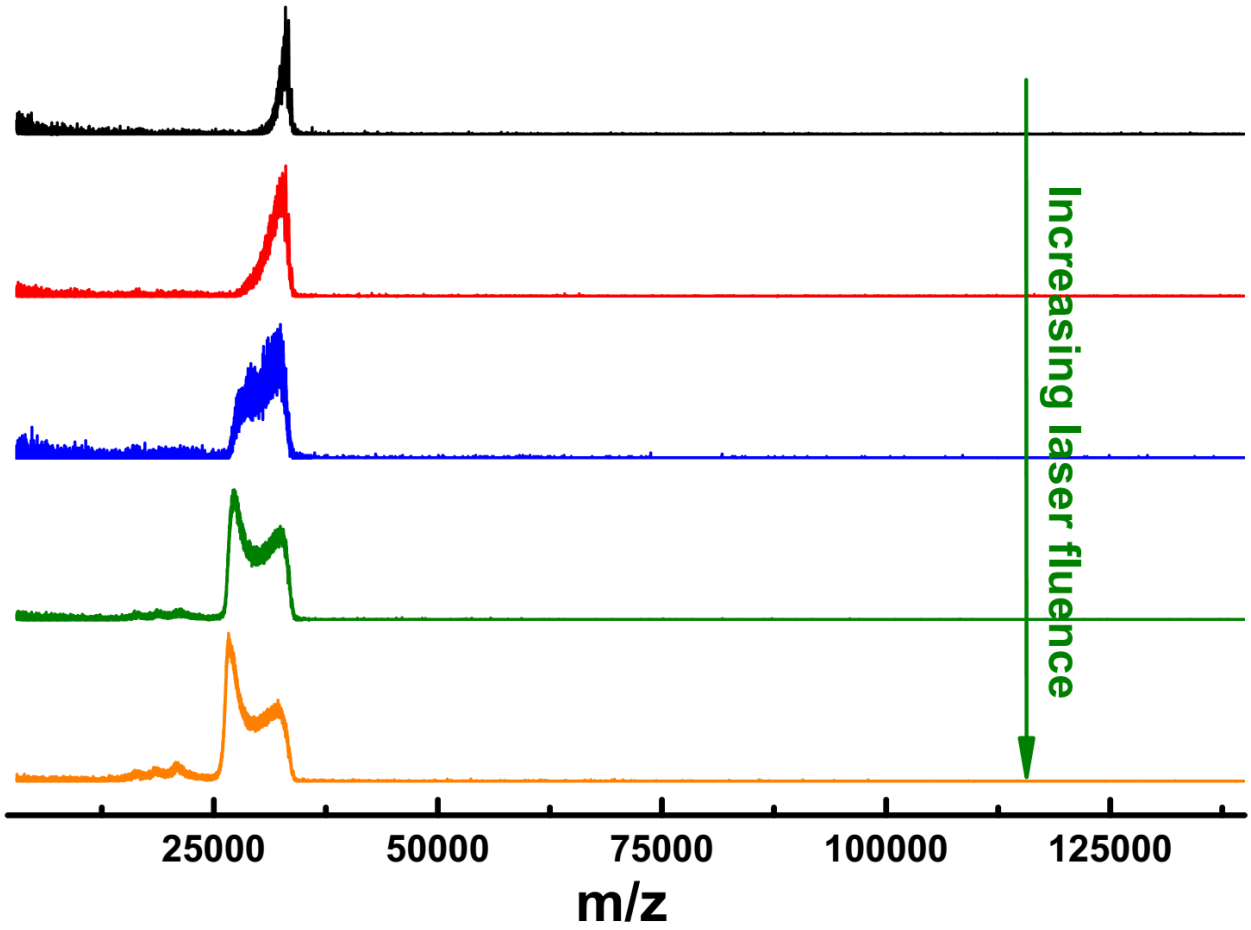


**Figure S4. MALDI-MS at very high laser fluence to demonstrate the absence of larger than 133-Au atom compounds.** Positive mode MALDI MS data obtained at varying laser fluence. High laser induces fragmentation of the nanomolecule while the low laser gives intact molecular ion. There are no peaks in the larger mass range even at very high laser fluence indicating the high purity of the sample.

MALDI MS data at high laser fluence is necessary to demonstrate the purity of the sample, because at lower laser fluence only smaller nanomolecules may ionize. Upon increasing the laser fluence from the top black spectrum to the bottom orange spectrum, no additional peaks corresponding to the larger nanoparticles are observed.

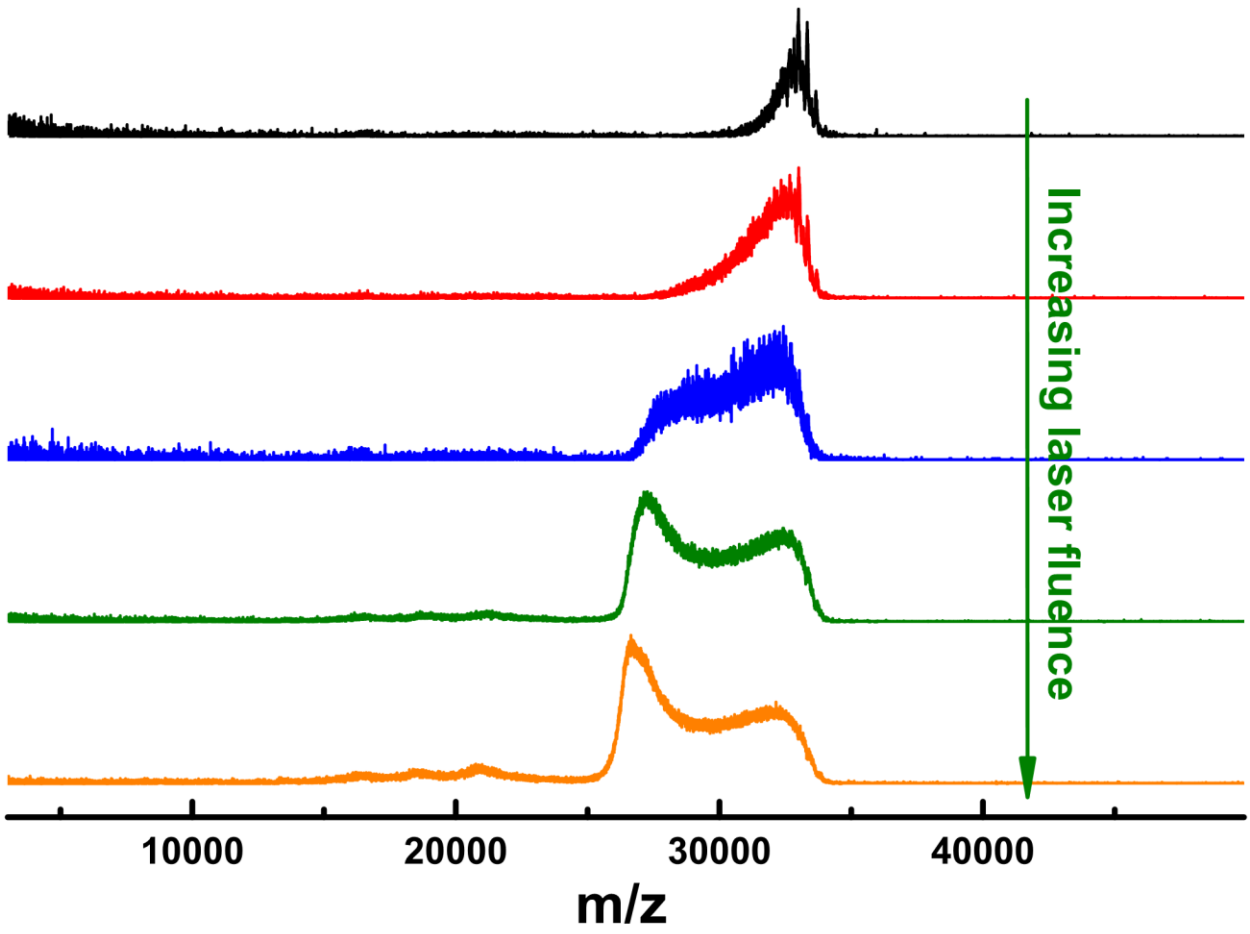


**Figure S5. MALDI-MS at varying laser fluence to show the fragmentation.** Positive mode MALDI MS data obtained at varying laser fluence. Same as the figure S4, but expanded in the mass range around the molecular ion of $Au_{133}(SPh\text{-}t\text{Bu})_{52}$, to show the fragmentation.

## 9. Small angle X-ray scattering (SAXS)

Solution x-ray scattering data were also collected for $Au_{133}(SPh\text{-}tBu)_{52}$ particles. The uniform size of the particles was demonstrated by the wide range of linear Guinier behavior (ln[*I*(q)] vs $q^2$), see Figure Sx. The pair distance distribution function derived from the x-ray scattering data exhibits a Gaussian-like profile, suggesting that Au133 particle adopts a spheroid shape. The largest dimension of the particle obtained from the PDDF is about 2.4 nm.

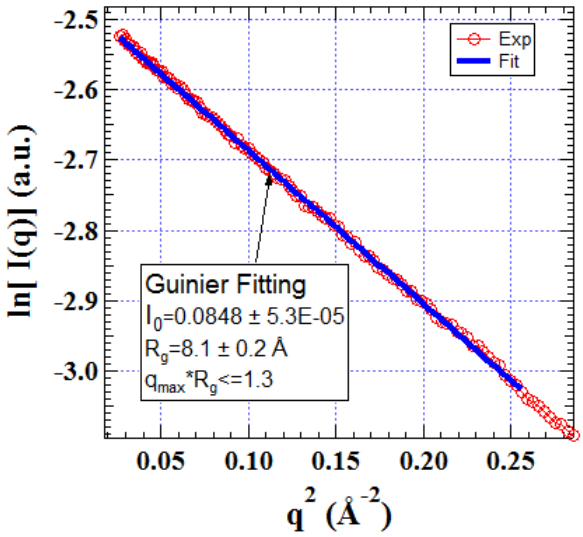


**Figure S6.** Fitting (blue line) for small-angle x-ray (SAXS) data (red open circles with error bar) of Au133 with Guinier equation: $\ln[I(q)] = \ln[\mathrm{Io}] - \frac{R_g^2 q^2}{3}$. The linear plot (ln[I(q)] vs $q^2$) indicates the high monodisperisity of the sample in size. The radius of gyration obtained from the fitting is 8.1 ± 0.2 Å.

## 10. TD-DFT and electronic structure analysis

The Projected Density of States (PDOS) of the $Au_{133}(SPh\text{-}tBu)_{52}$ cluster as projected onto Au, S, C and H atoms is shown in Fig. S7. An incipient metallic character of the system associated with a very small HOMO-LUMO gap can be appreciated, as discussed in the main text.

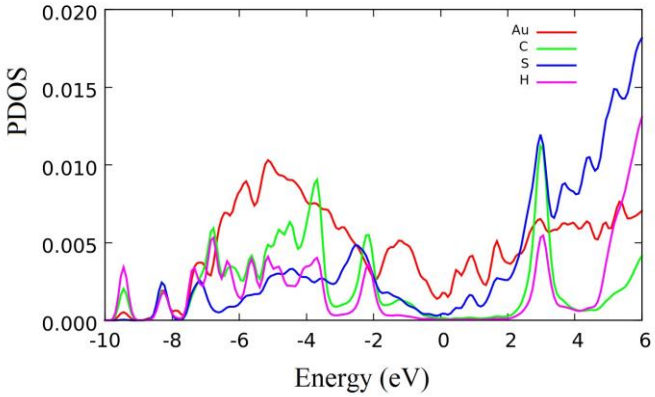


**Figure S7**. PDOS of the $Au_{133}(SPh\text{-}tBu)_{52}$ cluster as projected onto Au, S, C and H atoms.

In Fig. S8 TDDFT simulated spectra are reported. Fig.S8(left panel) shows a comparison of the TDDFT spectra of $Au_{133}(SPh)_{52}^{+1}$ along the three Cartesian directions.

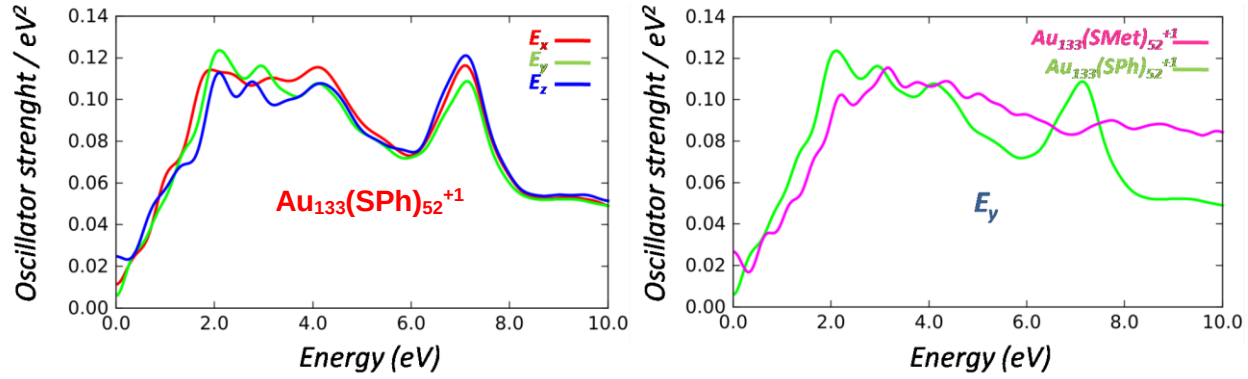


**Figure S8.** Left panel - absorption spectra of $Au_{133}(SC_6H_5)_{52}^{+1}$ probed by electrical pulses along the three Cartesian directions. Right panel - Comparison of the absorption spectra along the *y*-Cartesian direction of $Au_{133}(SPh)_{52}^{+1}$ (green) and $Au_{133}(SC_6H_5)_{52}^{+1}$ (magenta).

A comparison of the TDDFT spectra of $Au_{133}(SPh)_{52}^{+1}$ and $Au_{133}(SC_6H_5)_{52}^{+1}$ reported in the right panel of Fig.S8 is instructive: the conjugated nanomolecule exhibits a less fragmented absorption, in agreement with experiment. It is interesting to observe in passing that the $Au_{133}(SCH_3)_{52}$ spectrum is similar to that of $Au_{144}(SCH_2CH_2Ph)_{60}$.(*15*) Note that, to speed up TDDFT calculations, these were conducted on a $Au_{133}(SPh)_{52}$ compound in which the *p*-tBu ligands were replaced with hydrogen atoms (otherwise using the equilibrium geometry of the parent compound), but this does not alter their electronic (e.g., conjugating) characteristics. Finally, it should be added that the TDDFT calculations were performed on singly charged $Au_{133}(SPh\text{-}tBu)_{52}$ and $Au_{133}(SCH_3)_{52}$ cations to obtain electronically closed shell systems for reasons of computational convenience – a unit charge on a large cluster is however known not to affect optical response appreciably.

## 12. X-ray Crystallographic coordinates for Au133S52

**Table S2** Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for Au133S52_Mar26_1. $U_{eq}$ is defined as 1/3 of of the trace of the orthogonalised $U_{IJ}$ tensor.

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| Au(1) | 0 | -2113(1) | 7500 | 81(1) |
| Au(2) | -182(1) | -1503(1) | 7774(1) | 83(1) |
| Au(1A) | -416(1) | -3816(1) | 7523(1) | 102(1) |
| Au(1B) | -421(1) | -3330(1) | 8020(1) | 97(1) |
| Au(1C) | 281(1) | -2726(1) | 6558(1) | 90(1) |
| Au(1D) | 459(1) | -423(1) | 7479(1) | 99(1) |
| Au(1E) | 1395(1) | -2115(1) | 7700(1) | 101(1) |
| Au(1F) | 281(1) | -487(1) | 6301(1) | 117(1) |
| Au(1G) | 898(1) | -817(1) | 7138(1) | 102(1) |
| Au(1H) | 1134(1) | -1067(1) | 7745(1) | 103(1) |
| Au(1I) | 1679(1) | -1466(1) | 7756(1) | 111(1) |
| Au(3) | 375(1) | -1737(1) | 7866(1) | 84(1) |
| Au(4) | 537(1) | -2110(1) | 7288(1) | 85(1) |
| Au(5) | 84(1) | -2119(1) | 6827(1) | 83(1) |
| Au(6) | 193(1) | -2724(1) | 7238(1) | 85(1) |
| Au(7) | -367(1) | -2483(1) | 7117(1) | 87(1) |
| Au(8) | -917(1) | -2504(1) | 7321(1) | 92(1) |
| Au(9) | -583(1) | -3115(1) | 7384(1) | 91(1) |
| Au(10) | -730(1) | -2877(1) | 6739(1) | 95(1) |
| Au(11) | -189(1) | -3123(1) | 6848(1) | 93(1) |
| Au(12) | -291(1) | -2497(1) | 6424(1) | 91(1) |
| Au(13) | -752(1) | -2108(1) | 6742(1) | 90(1) |
| Au(14) | -746(1) | -2720(1) | 7975(1) | 90(1) |
| Au(15) | -300(1) | -1724(1) | 6447(1) | 90(1) |
| Au(16) | -393(1) | -2098(1) | 5875(1) | 101(1) |
| Au(17) | 631(1) | -2114(1) | 6600(1) | 91(1) |
| Au(18) | 146(1) | -2094(1) | 6132(1) | 94(1) |

| | | | | |
|---|---|---|---|---|
| Au(19) | 261(1) | -1510(1) | 6529(1) | 90(1) |
| Au(20) | 725(1) | -1500(1) | 7011(1) | 91(1) |
| Au(21) | 1098(1) | -2133(1) | 7102(1) | 98(1) |
| Au(22) | 930(1) | -1726(1) | 7661(1) | 92(1) |
| Au(23) | 563(1) | -1092(1) | 7607(1) | 91(1) |
| Au(24) | 187(1) | -1111(1) | 8177(1) | 89(1) |
| Au(25) | 743(1) | -1337(1) | 8228(1) | 93(1) |
| Au(26) | 0 | -882(1) | 7500 | 92(1) |
| Au(27) | 1115(1) | -913(1) | 8568(1) | 108(1) |
| Au(28) | 612(1) | -631(1) | 8133(1) | 101(1) |
| Au(29) | 449(1) | -503(1) | 8905(1) | 115(1) |
| Au(30) | 0 | -3345(1) | 7500 | 93(2) |
| Au(31) | 0 | 153(1) | 7500 | 124(2) |
| Au(32) | -41(1) | -407(1) | 7005(1) | 101(1) |
| Au(33) | -852(1) | -1701(1) | 6188(1) | 100(1) |
| Au(34) | 361(1) | -899(1) | 6908(1) | 94(1) |
| Au(35) | 1090(1) | -1735(1) | 6493(1) | 102(1) |
| Au(36) | -1223(1) | -2503(1) | 6705(1) | 102(1) |
| Au(37) | 1238(1) | -1790(1) | 8291(1) | 99(1) |
| Au(38) | -855(1) | -2414(1) | 6163(1) | 103(1) |
| Au(39) | -745(1) | -3099(1) | 8556(1) | 102(1) |
| Au(40) | 66(1) | -3794(1) | 8054(1) | 101(1) |
| Au(42) | -1086(1) | -3278(1) | 6346(1) | 112(1) |
| Au(43) | -627(1) | -3586(1) | 6858(1) | 105(1) |
| Au(45) | 1100(1) | -2468(1) | 6489(1) | 103(1) |
| Au(46) | 739(1) | -1144(1) | 6428(1) | 100(1) |
| Au(48) | 55(1) | -2813(1) | 5952(1) | 109(1) |
| Au(49) | 656(1) | -1774(1) | 6021(1) | 104(1) |
| Au(50) | 0 | -4377(1) | 7500 | 137(2) |
| Au(51) | 645(1) | -2504(1) | 6046(1) | 104(1) |
| Au(52) | -140(1) | -3402(1) | 8622(1) | 105(1) |
| Au(53) | 1260(1) | -1420(1) | 7165(1) | 103(1) |
| Au(57) | -533(1) | -3321(1) | 9195(1) | 115(1) |
| Au(59) | -1119(1) | -3090(1) | 7634(1) | 106(1) |
| Au(61) | -406(1) | -3156(1) | 6193(1) | 106(1) |
| Au(62) | 1295(1) | -913(1) | 6549(1) | 117(1) |

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|---|---|---|---|---|
| Au(64) | -89(1) | -1150(1) | 6139(1) | 103(1) |
| Au(65) | 1564(1) | -2613(1) | 7070(1) | 120(1) |
| Au(66) | -492(1) | -2734(1) | 5542(1) | 119(1) |
| Au(67) | -1211(1) | -3714(1) | 7189(1) | 126(1) |
| Au(68) | -924(1) | -3750(1) | 8038(1) | 116(1) |
| Au(69) | 137(1) | -1629(1) | 5564(1) | 121(1) |
| S(1) | 972(5) | -1165(6) | 9058(6) | 111(8) |
| S(2) | 576(6) | -809(6) | 5978(6) | 115(8) |
| S(1A) | 476(7) | 184(6) | 7383(7) | 143(11) |
| S(1B) | 1093(6) | -419(6) | 6745(6) | 120(8) |
| S(3) | -755(6) | -3568(6) | 6060(6) | 131(10) |
| S(4) | -43(7) | -2694(6) | 5398(5) | 142(12) |
| S(5) | 31(6) | -44(6) | 6540(5) | 117(8) |
| S(6) | -338(7) | -1729(7) | 5415(6) | 149(11) |
| S(7) | 1643(5) | -1451(6) | 8326(5) | 110(8) |
| S(8) | -955(6) | -2734(6) | 5665(6) | 120(9) |
| S(9) | -400(6) | -3828(7) | 8928(6) | 132(9) |
| S(10) | 684(7) | -2823(6) | 5541(6) | 135(10) |
| S(11) | -1468(5) | -3021(5) | 6594(6) | 110(8) |
| S(12) | 600(6) | -1490(6) | 5508(6) | 120(8) |
| S(13) | 1493(6) | -1417(6) | 6374(6) | 121(8) |
| S(14) | 652(5) | -169(6) | 8512(6) | 118(8) |
| S(15) | 1737(6) | -1519(6) | 7196(6) | 122(8) |
| S(16) | -1133(6) | -3465(6) | 8458(6) | 127(9) |
| S(17) | 1758(6) | -2509(6) | 7573(7) | 133(9) |
| S(18) | 10(6) | -4401(6) | 8081(8) | 141(10) |
| S(21) | -957(7) | -4056(6) | 6866(6) | 140(11) |
| S(30) | -791(5) | -4188(6) | 7691(7) | 121(9) |
| S(36) | 1549(7) | -2774(6) | 6514(7) | 138(10) |
| S(65) | -1519(6) | -3393(6) | 7464(6) | 123(9) |
| S(70) | -304(5) | -860(6) | 5680(6) | 116(8) |
| S(96) | 1289(5) | -630(6) | 8103(6) | 110(8) |
| C(1) | 2089(10) | -2292(15) | 7504(18) | 128(18) |
| C(2) | 2218(14) | -2128(16) | 7769(12) | 132(18) |
| C(3) | 2476(14) | -1983(15) | 7728(13) | 133(18) |
| C(4) | 2606(9) | -2000(15) | 7423(17) | 116(16) |

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|---|---|---|---|---|
| C(5) | 2477(13) | -2163(15) | 7158(12) | 105(17) |
| C(6) | 2219(13) | -2309(14) | 7199(14) | 116(17) |
| C(7) | 2935(11) | -1880(20) | 7376(19) | 126(19) |
| C(8) | 2990(20) | -1860(30) | 7002(19) | 150(30) |
| C(11) | 1945(13) | -1686(19) | 8491(16) | 140(20) |
| C(12) | 2204(17) | -1535(13) | 8485(16) | 140(20) |
| C(13) | 2433(12) | -1720(20) | 8592(17) | 142(19) |
| C(14) | 2402(13) | -2054(19) | 8704(17) | 156(18) |
| C(15) | 2143(18) | -2205(13) | 8710(16) | 150(20) |
| C(16) | 1915(12) | -2021(19) | 8603(17) | 140(20) |
| C(17) | 2683(16) | -2300(20) | 8736(18) | 170(20) |
| C(18) | 2570(30) | -2640(20) | 8890(30) | 200(40) |
| C(19) | 2760(30) | -2020(20) | 8990(30) | 200(40) |
| C(21) | -688(14) | -4529(16) | 7977(16) | 125(19) |
| C(22) | -719(14) | -4860(20) | 7866(13) | 140(20) |
| C(23) | -656(15) | -5138(13) | 8074(19) | 150(20) |
| C(24) | -561(15) | -5075(16) | 8394(17) | 150(20) |
| C(25) | -530(14) | -4740(20) | 8505(13) | 140(20) |
| C(26) | -593(15) | -4467(14) | 8297(18) | 140(20) |
| C(31) | -50(10) | -668(16) | 5415(14) | 112(17) |
| C(32) | 76(13) | -356(15) | 5489(12) | 113(17) |
| C(33) | 286(13) | -233(13) | 5289(17) | 133(18) |
| C(34) | 370(11) | -421(18) | 5015(15) | 144(17) |
| C(35) | 244(14) | -732(17) | 4942(12) | 134(18) |
| C(36) | 34(13) | -856(12) | 5142(16) | 121(18) |
| C(37) | 615(12) | -350(16) | 4730(13) | 150(19) |
| C(38) | 680(20) | 9(18) | 4860(20) | 170(30) |
| C(39) | 485(18) | -350(20) | 4383(18) | 140(30) |
| C(40) | 847(19) | -610(20) | 4780(20) | 180(30) |
| C(41) | -1147(13) | -3796(15) | 8791(13) | 122(18) |
| C(42) | -1198(14) | -3672(11) | 9107(17) | 129(18) |
| C(43) | -1218(14) | -3898(18) | 9371(11) | 128(18) |
| C(44) | -1188(14) | -4249(16) | 9319(14) | 138(17) |
| C(45) | -1138(14) | -4373(11) | 9003(17) | 133(18) |
| C(46) | -1118(13) | -4146(17) | 8738(11) | 126(18) |
| C(47) | -1241(14) | -4502(15) | 9650(13) | 160(20) |

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|---|---|---|---|---|
| C(48) | -1130(19) | -4850(20) | 9540(20) | 170(30) |
| C(49) | -1554(15) | -4490(30) | 9700(30) | 180(30) |
| C(50) | -1075(19) | -4340(20) | 9930(20) | 190(30) |
| C(51) | -1124(14) | -2476(16) | 5356(14) | 128(19) |
| C(52) | -1185(14) | -2131(17) | 5402(11) | 127(18) |
| C(53) | -1272(13) | -1932(12) | 5136(17) | 123(18) |
| C(54) | -1299(13) | -2078(17) | 4824(13) | 134(17) |
| C(55) | -1238(14) | -2423(18) | 4778(12) | 136(18) |
| C(56) | -1151(14) | -2622(12) | 5044(17) | 134(19) |
| C(57) | -1473(12) | -1868(15) | 4528(14) | 147(19) |
| C(58) | -1543(19) | -1540(20) | 4720(20) | 150(30) |
| C(59) | -1721(16) | -2080(20) | 4410(20) | 160(30) |
| C(60) | -1240(16) | -1840(30) | 4280(20) | 180(30) |
| C(61) | -1659(14) | -2976(19) | 6191(12) | 131(19) |
| C(62) | -1595(12) | -2710(15) | 5976(18) | 125(19) |
| C(63) | -1728(15) | -2685(15) | 5672(15) | 130(19) |
| C(64) | -1925(14) | -2930(20) | 5583(13) | 147(18) |
| C(65) | -1989(13) | -3193(17) | 5798(19) | 160(20) |
| C(66) | -1856(15) | -3218(15) | 6102(17) | 140(20) |
| C(67) | -2070(20) | -2890(20) | 5202(16) | 150(20) |
| C(68) | -1950(20) | -3230(20) | 5050(20) | 150(30) |
| C(71) | 1321(11) | -1196(19) | 9255(16) | 126(19) |
| C(72) | 1515(16) | -1433(15) | 9149(14) | 138(19) |
| C(73) | 1783(14) | -1417(16) | 9268(17) | 146(19) |
| C(74) | 1857(11) | -1160(20) | 9494(17) | 144(18) |
| C(75) | 1663(16) | -926(15) | 9600(14) | 137(19) |
| C(76) | 1395(13) | -942(15) | 9480(16) | 133(19) |
| C(77) | 2194(12) | -1240(20) | 9560(30) | 150(20) |
| C(78) | 2340(20) | -960(20) | 9360(20) | 150(30) |
| C(79) | 2160(30) | -1100(30) | 9940(20) | 200(30) |
| C(81) | 716(17) | -1720(20) | 5175(19) | 170(20) |
| C(82) | 777(18) | -2070(30) | 5201(17) | 180(20) |
| C(83) | 826(17) | -2262(16) | 4920(30) | 180(20) |
| C(84) | 814(17) | -2110(30) | 4608(19) | 180(20) |
| C(85) | 753(18) | -1760(30) | 4582(17) | 190(20) |
| C(86) | 704(17) | -1567(16) | 4870(30) | 180(20) |

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|---|---|---|---|---|
| C(87) | 960(20) | -2330(30) | 4300(20) | 180(20) |
| C(88) | 1170(20) | -2130(30) | 4090(30) | 180(30) |
| C(91) | 1966(15) | -1149(16) | 7068(15) | 140(20) |
| C(92) | 2235(16) | -1223(13) | 6977(16) | 135(19) |
| C(93) | 2396(11) | -970(20) | 6829(16) | 139(19) |
| C(94) | 2288(15) | -646(17) | 6773(16) | 149(19) |
| C(95) | 2019(17) | -573(13) | 6864(17) | 150(20) |
| C(96) | 1858(11) | -820(20) | 7011(16) | 140(20) |
| C(97) | 2470(20) | -320(20) | 6620(30) | 160(30) |
| C(101) | 994(10) | -44(17) | 8633(17) | 127(19) |
| C(102) | 1081(13) | -140(15) | 8948(16) | 122(18) |
| C(103) | 1343(15) | -52(16) | 9058(12) | 131(18) |
| C(104) | 1518(10) | 131(17) | 8853(18) | 143(17) |
| C(105) | 1432(14) | 226(15) | 8538(17) | 136(19) |
| C(106) | 1170(16) | 139(17) | 8428(12) | 140(19) |
| C(107) | 1811(12) | 316(19) | 8986(19) | 160(20) |
| C(108) | 1930(20) | 400(20) | 8640(20) | 150(30) |
| C(109) | 1940(20) | 0(30) | 9150(20) | 180(30) |
| C(111) | -1150(16) | -4135(17) | 6490(14) | 130(20) |
| C(112) | -1425(16) | -4046(16) | 6458(16) | 140(20) |
| C(113) | -1575(11) | -4158(19) | 6180(20) | 150(20) |
| C(114) | -1449(17) | -4358(19) | 5944(15) | 160(20) |
| C(115) | -1174(17) | -4447(16) | 5977(15) | 150(20) |
| C(116) | -1024(11) | -4335(18) | 6250(19) | 130(20) |
| C(117) | -1650(20) | -4470(30) | 5620(20) | 180(30) |
| C(121) | -322(17) | -1939(16) | 5027(13) | 130(20) |
| C(122) | -564(13) | -2095(18) | 4922(18) | 140(20) |
| C(123) | -582(13) | -2233(17) | 4610(20) | 150(20) |
| C(124) | -358(18) | -2216(17) | 4394(13) | 150(20) |
| C(125) | -116(14) | -2061(18) | 4499(17) | 150(20) |
| C(126) | -98(12) | -1922(16) | 4815(19) | 140(20) |
| C(131) | 1341(12) | -169(14) | 6949(16) | 115(18) |
| C(132) | 1503(14) | 48(17) | 6759(11) | 122(18) |
| C(133) | 1666(12) | 295(15) | 6911(17) | 137(18) |
| C(134) | 1667(13) | 325(15) | 7254(17) | 146(17) |
| C(135) | 1504(14) | 108(17) | 7444(11) | 126(18) |

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|---|---|---|---|---|
| C(136) | 1341(12) | -139(15) | 7291(15) | 124(18) |
| C(137) | 1914(17) | 520(20) | 7480(20) | 150(20) |
| C(138) | 2020(30) | 810(30) | 7250(30) | 180(30) |
| C(141) | 290(17) | -4662(18) | 8270(30) | 180(30) |
| C(142) | 490(20) | -4780(20) | 8048(16) | 190(30) |
| C(143) | 681(17) | -5020(20) | 8150(20) | 200(30) |
| C(144) | 677(17) | -5143(19) | 8470(30) | 200(30) |
| C(145) | 480(20) | -5030(20) | 8694(16) | 190(30) |
| C(146) | 286(17) | -4790(20) | 8590(20) | 180(30) |
| C(151) | 301(13) | 262(15) | 6595(14) | 120(18) |
| C(152) | 583(15) | 202(13) | 6603(14) | 121(18) |
| C(153) | 766(10) | 476(19) | 6613(15) | 133(19) |
| C(154) | 666(14) | 811(15) | 6614(15) | 133(19) |
| C(155) | 385(16) | 871(12) | 6607(15) | 141(19) |
| C(156) | 202(10) | 597(19) | 6597(15) | 131(19) |
| C(161) | 1540(15) | -1415(19) | 5937(12) | 134(19) |
| C(162) | 1419(12) | -1648(16) | 5721(19) | 140(20) |
| C(163) | 1500(15) | -1658(16) | 5392(17) | 138(19) |
| C(164) | 1703(16) | -1440(20) | 5279(12) | 148(18) |
| C(165) | 1824(13) | -1203(16) | 5495(19) | 146(19) |
| C(166) | 1743(14) | -1193(15) | 5824(17) | 140(20) |
| C(167) | 1760(20) | -1410(30) | 4868(14) | 160(20) |
| C(168) | 2040(20) | -1220(30) | 4850(30) | 190(30) |
| C(171) | -156(14) | -4058(15) | 9187(15) | 129(19) |
| C(172) | -253(10) | -4250(17) | 9452(17) | 124(18) |
| C(173) | -71(15) | -4438(15) | 9646(13) | 142(19) |
| C(174) | 208(13) | -4434(16) | 9576(16) | 138(17) |
| C(175) | 306(10) | -4242(18) | 9311(18) | 140(19) |
| C(176) | 124(16) | -4054(16) | 9117(13) | 142(19) |
| C(177) | 481(11) | -4640(15) | 9737(15) | 152(19) |
| C(178) | 394(18) | -5008(19) | 9650(20) | 140(30) |
| C(179) | 776(15) | -4550(20) | 9630(20) | 170(30) |
| C(180) | 408(19) | -4530(20) | 10092(19) | 160(30) |
| C(181) | 55(16) | -3050(20) | 5116(19) | 170(20) |
| C(182) | 79(16) | -3390(20) | 5184(15) | 160(20) |
| C(183) | 181(17) | -3616(15) | 4940(20) | 170(20) |

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|---|---|---|---|---|
| C(184) | 258(16) | -3490(20) | 4640(20) | 180(20) |
| C(185) | 233(17) | -3140(20) | 4569(16) | 180(20) |
| C(186) | 132(17) | -2919(15) | 4810(20) | 180(20) |
| C(187) | 340(30) | -3850(20) | 4430(30) | 190(30) |
| C(191) | 1664(10) | -598(16) | 8129(19) | 133(19) |
| C(192) | 1794(15) | -572(16) | 7824(14) | 126(19) |
| C(193) | 2079(15) | -541(16) | 7810(14) | 134(19) |
| C(194) | 2233(10) | -535(17) | 8100(20) | 145(19) |
| C(195) | 2103(15) | -561(17) | 8404(15) | 140(19) |
| C(196) | 1819(16) | -592(17) | 8419(13) | 140(19) |
| C(197) | 2579(11) | -530(30) | 8090(30) | 150(30) |
| C(201) | -827(16) | -3594(16) | 5635(11) | 128(19) |
| C(202) | -621(11) | -3553(16) | 5401(19) | 129(19) |
| C(203) | -685(14) | -3562(17) | 5066(16) | 141(19) |
| C(204) | -956(17) | -3612(17) | 4964(12) | 148(18) |
| C(205) | -1162(11) | -3652(17) | 5200(20) | 147(19) |
| C(206) | -1097(14) | -3644(17) | 5533(17) | 141(19) |
| C(207) | -997(19) | -3670(20) | 4555(12) | 150(20) |
| C(208) | -1226(18) | -3410(30) | 4490(30) | 170(30) |
| C(209) | -762(17) | -3660(30) | 4300(20) | 150(30) |
| C(211) | -1674(17) | -3650(20) | 7787(16) | 170(20) |
| C(212) | -1863(18) | -3473(15) | 7980(20) | 160(20) |
| C(213) | -1972(15) | -3630(20) | 8260(20) | 180(20) |
| C(214) | -1893(18) | -3970(20) | 8342(16) | 180(20) |
| C(215) | -1704(18) | -4138(15) | 8140(20) | 170(20) |
| C(216) | -1595(15) | -3980(20) | 7870(20) | 170(20) |
| C(217) | -2010(30) | -4150(30) | 8690(20) | 200(40) |
| C(221) | 640(20) | 449(18) | 7709(18) | 160(20) |
| C(222) | 887(18) | 630(20) | 7681(17) | 180(20) |
| C(223) | 978(13) | 830(20) | 7940(30) | 180(20) |
| C(224) | 820(20) | 868(18) | 8222(19) | 180(20) |
| C(225) | 574(18) | 690(20) | 8250(16) | 170(20) |
| C(226) | 483(13) | 483(19) | 7990(20) | 160(20) |
| C(227) | 900(20) | 1202(19) | 8470(20) | 190(20) |
| C(228) | 900(30) | 1010(30) | 8800(30) | 200(40) |
| C(229) | 1190(30) | 1270(40) | 8330(30) | 230(40) |

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|---|---|---|---|---|
| C(231) | 850(14) | -540(20) | 5829(16) | 150(20) |
| C(232) | 839(14) | -190(20) | 5833(16) | 150(20) |
| C(233) | 1057(19) | 5(13) | 5709(18) | 160(20) |
| C(234) | 1286(15) | -160(20) | 5581(17) | 165(19) |
| C(235) | 1298(13) | -520(20) | 5577(17) | 160(20) |
| C(236) | 1080(19) | -708(13) | 5701(18) | 150(20) |
| C(237) | 1534(16) | 110(20) | 5449(19) | 170(20) |
| C(238) | 1460(20) | 470(30) | 5570(30) | 190(30) |
| C(239) | 1790(20) | -40(30) | 5620(30) | 190(30) |
| C(241) | 1046(13) | -2910(20) | 5420(20) | 150(20) |
| C(242) | 1111(17) | -3127(18) | 5156(19) | 150(20) |
| C(243) | 1380(20) | -3164(17) | 5059(15) | 160(20) |
| C(244) | 1591(13) | -2990(20) | 5230(20) | 170(20) |
| C(245) | 1525(17) | -2770(20) | 5490(20) | 170(20) |
| C(246) | 1250(20) | -2738(17) | 5587(15) | 160(20) |
| C(251) | 1841(14) | -2530(20) | 6340(20) | 130(30) |

## 13. Coordinates from DFT calculations for $Au_{133}(SPh\text{-}tBu)_{52}$

1381

| | | | |
|---|---|---|---|
| Au | 20.0000000000 | 20.0000000000 | 20.0000000000 |
| Au | 18.2414113879 | 19.0566387326 | 21.9293403476 |
| Au | 19.7587678581 | 17.2567523867 | 20.2430622727 |
| Au | 17.5906718373 | 18.8957818300 | 19.1749031991 |
| Au | 21.1440340877 | 18.8880470544 | 22.2411256880 |
| Au | 17.7200813890 | 21.5046641976 | 20.4248980135 |
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