

## Supporting Information

### **Au<sub>279</sub>(SR)<sub>84</sub>: The Smallest Gold Thiolate Nanocrystal that is Metallic and the Birth of Plasmon.**

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## 1. Experimental section

**Materials.** Hydrogen tetrachloroaurate (III) ( $\text{HAuCl}_4 \cdot 3\text{H}_2\text{O}$ ) (Alfa Aesar ACS grade), tetraoctylammonium bromide (TOABr) (Acros), sodium borohydride ( $\text{NaBH}_4$ ) (Acros, 99%), *tert*-butyl benzene thiol, (TBBT) (TCI America, >97%), anhydrous ethyl alcohol (Acros, 99.5%), and trans-2-[3[(4-*tert*butyl-phenyl)-2-methyl-2-propenylidene] malononitrile (DCTB matrix) (Fluka $\geq$ 99%) were used as received. HPLC grade solvents ethyl acetate (EtOAc), methylene chloride (DCM), tetrahydrofuran (THF), toluene, methanol, butylated hydroxytoluene stabilized tetrahydrofuran (THF-BHT) and acetonitrile were purchased from Fisher Scientific. All materials were used as received.

**Synthesis.**  $\text{Au}_{36}(\text{TBBT})_{24}$  and  $\text{Au}_{44}(\text{TBBT})_{28}$  were synthesized following a previous report<sup>1</sup> yielding a mixture of nanomolecules containing  $\text{Au}_{36}(\text{SR})_{24}$ , and  $\text{Au}_{44}(\text{SR})_{28}$ . AuNMs were isolated from the mixture by performing size exclusion chromatography (SEC)<sup>2</sup> using Bio-Rad SX1 support beads, and THF-BHT as a solvent. Briefly, 50 mg  $\text{HAuCl}_4 \cdot 3\text{H}_2\text{O}$  was dissolved in 10 ml THF (15 mM) and reacted with 4-*tert*butylbenzenethiol (TBBT) ( $\text{Au}:\text{thiol} = 1:5$ ) for 30 minutes (stir, 500 rpm). Then, the reaction mixture was reduced with  $\text{NaBH}_4$  ( $\text{Au}:\text{NaBH}_4 = 1:10$ ) dissolved in water (5 ml). The reaction was stopped after 5 minutes, and the solvent was removed by rotary evaporation. The crude product was purified by washing with methanol. The crude product was thermochemically treated with excess thiol at 80 °C for 1 day. The reaction mixture was washed with methanol to remove excess thiols.

$\text{Au}_{133}$ :  $\text{Au}_{133}(\text{TBBT})_{52}$  was synthesized by core-conversion of  $\text{Au}_{144}(\text{SCH}_2\text{CH}_2\text{Ph})_{60}$  using the reported protocol.<sup>3</sup>

*F-279*:  $\text{Au}_{279}(\text{TBBT})_{84}$  nanocrystals were synthesized using the reported protocol.<sup>4</sup>

**Instrumentation.** Room temperature optical UV–Vis–NIR absorption data were collected using Shimadzu UV-1601 spectrophotometer with toluene as the solvent at very slow scan rate. Differential pulse voltammetry (DPV) measurement was performed on a CHI 620 instrument in anhydrous 1,2-dichloroethane with 0.5 mM bis(triphenylphosphoranylidene) ammonium tetrakis(pentafluorophenyl) borate [ $\text{BTPPATBF}_{20}$ ] as supporting electrolyte under nitrogen atmosphere. A three electrode setup with Pt working electrode, Pt wire counter electrode and Ag/AgCl reference electrode were used. DPV was performed at a scan rate of 6 mV/s, pulse height of 0.05 V, pulse width of 0.2 s and pulse period of 0.05 s.

**2. Computational details and further discussion.** The experimental X-ray  $\text{Au}_{279}\text{S}_{84}$  core geometry was completed by adding 84 Ph residues to obtain a  $\text{Au}_{279}(\text{SPh})_{84}$  model (the *tert*-butyl groups of the experimental compound were simplified with hydrogen atoms to reduce computational effort). This model was subjected to local geometry relaxation followed by two 0.5-ps runs of Molecular Dynamics (MD) at 300 K, and a final local geometry relaxation (the experimental  $\text{Au}_{279}\text{S}_{84}$  core was kept frozen in all simulations). We employed a density-functional tight binding (DFTB-D3) approach<sup>5</sup> including dispersion terms in the Grimme-D3 formalism<sup>6</sup> in both geometry relaxations and MD runs. Constrained MD runs were performed using a time-step of 0.5 fs in a NVT ensemble whose temperature was controlled by a Nose-Hoover thermostat.<sup>7</sup> The DFTB Slater–Koster files were taken from Ref.<sup>8</sup>. An identical procedure was used to generate a  $\text{Au}_{279}(\text{SCH}_3)_{84}$  model for comparison purposes. The Cartesian coordinates of these structural models are reported below. On these geometries standard DFT calculations were also performed using two exchange correlation (xc-) functionals and the ADF code<sup>9</sup>: the Local Density Approximation (LDA)<sup>10</sup> and the vanLeeuwen-Baerends<sup>11</sup> one (LB94) which supports an

asymptotically correct Coulombic tail of the xc-potential to improve the description of the band gap and virtual orbitals. From these simulations plots the Projected Density Of States (PDOS) of the systems were extracted, using a Lorentzian smooth with full width at half maximum (FWHM) set to 0.12 eV.

Optical absorption spectra were simulated on the final optimized geometries via a real-time time-dependent density functional theory (RT-TDDFT) approach<sup>12</sup> employing the CP2K code<sup>13</sup> and using the Perdew–Burke–Ernzerhof (PBE) xc-functional<sup>14</sup> and a hybrid Gaussian/Plane-Wave scheme (GPW)<sup>15</sup> in which DZVP basis sets<sup>16</sup> plus GTH pseudopotentials<sup>17</sup> were used to represent the DFT Kohn–Sham orbitals, while the cut-off for the auxiliary plane wave representation of the density was set to 300 Ry. In the RT-TDDFT approach, optical response was obtained by subjecting the system to electrical pulses of strength 0.005 a.u in each of the three Cartesian directions, and then following the electron dynamics for a total of 9 femto-seconds sampling the time-interval with time steps of 0.012 fs. A time damping of 7.2 fs (corresponding to a FWHM of 0.25 eV) was chosen to broaden the simulated spectrum. The adopted procedure is identical to the one previously employed in Ref.<sup>18</sup> to simulate the optical spectrum of Au<sub>133</sub>(SPh)<sub>52</sub>, thus allowing us a one-to-one comparison between the two systems, despite the limitations in the description of electronic structure associated with the use of the PBE xc-functional, which is here adopted for reasons of computational feasibility but unfortunately lacks Hartree-Fock exchange and Coulombic-tail terms in the potential, thus underestimating the Coulomb couplings leading to a fully developed plasmonic resonance as previously observed in bare metal nanoclusters<sup>19</sup>.

Finally, to confirm the decisive contribution of the resonance/conjugation between the Au-S shell and the aromatic residues of the ligand to the plasmonic peak, we report that at the position of the plasmonic peak maximum (2 eV) a Mulliken charge analysis of the induced density obtained via the RT-TDDFT/PBE approach shows the following results:  $\delta q(\text{Au}) = -0.342$ ,  $\delta q(\text{S}) = -0.735$ ,  $\delta q(\text{CH}) = 1.052$ , for Au<sub>279</sub>(SPh)<sub>84</sub>, and  $\delta q(\text{Au}) = 0.303$ ,  $\delta q(\text{S}) = -0.266$ , and  $\delta q(\text{CH}) = -0.040$  for Au<sub>279</sub>(SCH<sub>3</sub>)<sub>84</sub>. This strongly support the case that the Ph residues receive charge from both Au and S in the plasmonic excited states.

The insurgence of a plasmon resonance in Au<sub>279</sub>(SPh)<sub>84</sub>, and the importance of ligand conjugation effects are fully confirmed and put on stronger grounds by exploratory RT-TDFT simulations using the VS98 xc-functional,<sup>20-21</sup> which has been shown to provide a better description of plasmonic effects<sup>22</sup>. From these simulations, whose results are shown in Figure S7 for the z-Cartesian component of the electric field only, it can be appreciated that Au<sub>279</sub>(SPh)<sub>84</sub> exhibits a clear plasmonic peak, much stronger than Au<sub>279</sub>(SCH<sub>3</sub>)<sub>84</sub>, (importance of ligand conjugation effects) or Au<sub>133</sub>(SPh)<sub>52</sub> (importance of size effects), or Au<sub>133</sub>(SCH<sub>3</sub>)<sub>52</sub> (importance of ligand conjugation effects).

### 3. Transient absorption measurements

Femtosecond transient absorption measurements were carried out at the Center for Nanoscale Materials, Argonne National Laboratory.<sup>20</sup> Briefly, a Spectra Physics Tsunami Ti:sapphire, 75 MHz oscillator was used to seed a 5 KHz Spectra-physics Spit-Fire Pro regenerative amplifier. 95% of the output from the amplifier is used to pump a TOPAS optical parametric amplifier, which is used to provide the pump beam in a Helios transient absorption setup (Ultrafast Systems Inc.). A pump beam of 370 nm was used for the measurements. The remaining 5% of the amplified output is focused onto a sapphire crystal to create a white light continuum that serves as the probe beam in our measurements (440 to 780 nm). The pump beam was depolarized and chopped at 2.5 kHz and both pump and probe beams were overlapped in the sample. Optical absorption spectra were taken before and after the measurements and the clusters have shown little degradation.

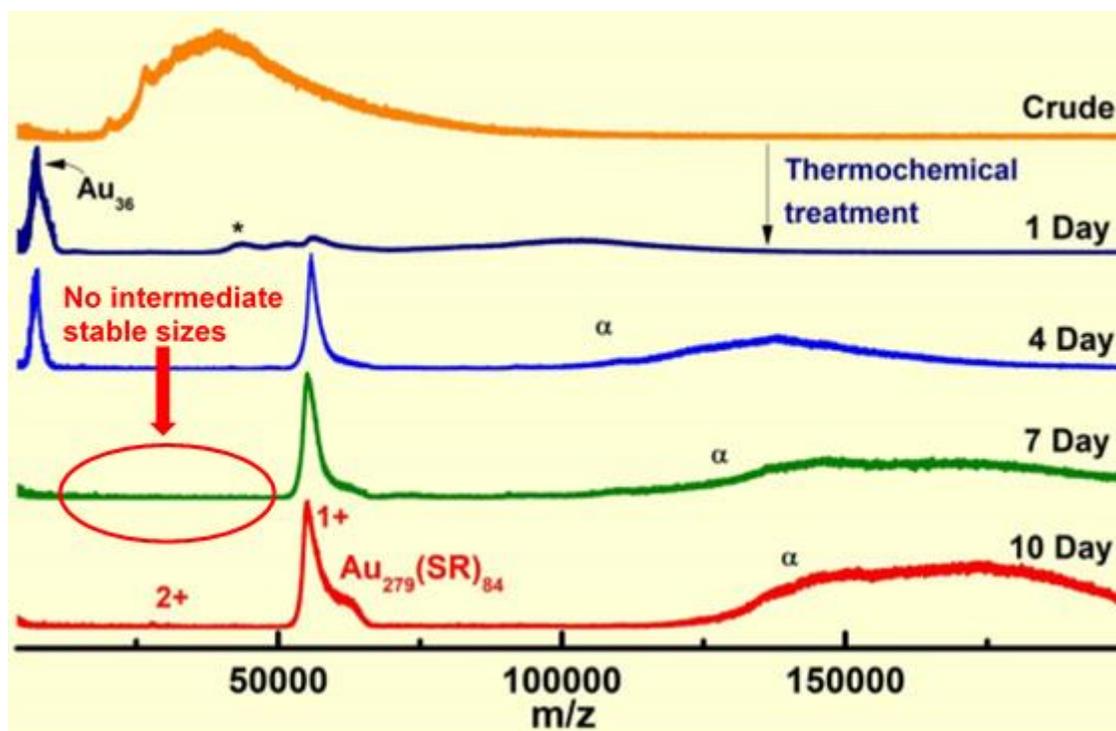
Nanosecond transient absorption measurements were carried out in an EOS transient absorption spectrometer with 370 nm as the excitation and a picosecond fiber optic continuum laser as the probe. All the data analysis was carried out using Surface Xplorer from Ultrafast Systems.

**4. Relationship between optical gap and lifetime of the electronically excited states.** The optical bandgap decreases as the size increases; Au<sub>36</sub> – 1.7 eV, and Au<sub>44</sub> – 1.5 eV. The electrochemical gap for Au<sub>36</sub> and Au<sub>44</sub> are 1.98 V and 1.65 V, respectively.<sup>23</sup> The electrochemical gap is larger than the optical gap for the two NMs due to the solution phase charging energy term. However, interpreting the optical gap based on absorption onset for larger NMs with onset energy <1 eV would lead to erroneous assessment.<sup>24</sup> HOMO-LUMO gap estimate for larger NMs can be obtained by differential pulse voltammetry studies. As the size increases, larger NMs exhibit quantized double layer (QDL) charging. Au<sub>133</sub> exhibits a QDL charging in voltammetry indicating the lack of bandgap with a peak spacing of ~0.2 V, the electronic density of states (DOS) reveals a bandgap of 0.05 eV and 0.11 eV for charge states of 0 and 1+, respectively.<sup>18</sup> DOS reveals that [Au<sub>279</sub>(SPh)<sub>84</sub>]<sup>+</sup> and [Au<sub>279</sub>(SCH<sub>3</sub>)<sub>84</sub>]<sup>+</sup> has a HOMO-LUMO gap of 0.083 eV and 0.087 eV, respectively. Voltammetry of Au<sub>279</sub> exhibits a QDL charging redox wave indicative of no band gap with a peak spacing of ~0.15 V (Figure S8). The DOS based gap of cationic Au<sub>279</sub> is less than that of Au<sub>133</sub> and follows the trend of decrease in band gap with increase in size. The excited state lifetimes also follow the same trend as band gap and reduces with increase in size. Figure S9 illustrates the trend observed in optical gap and lifetimes as the size increases.

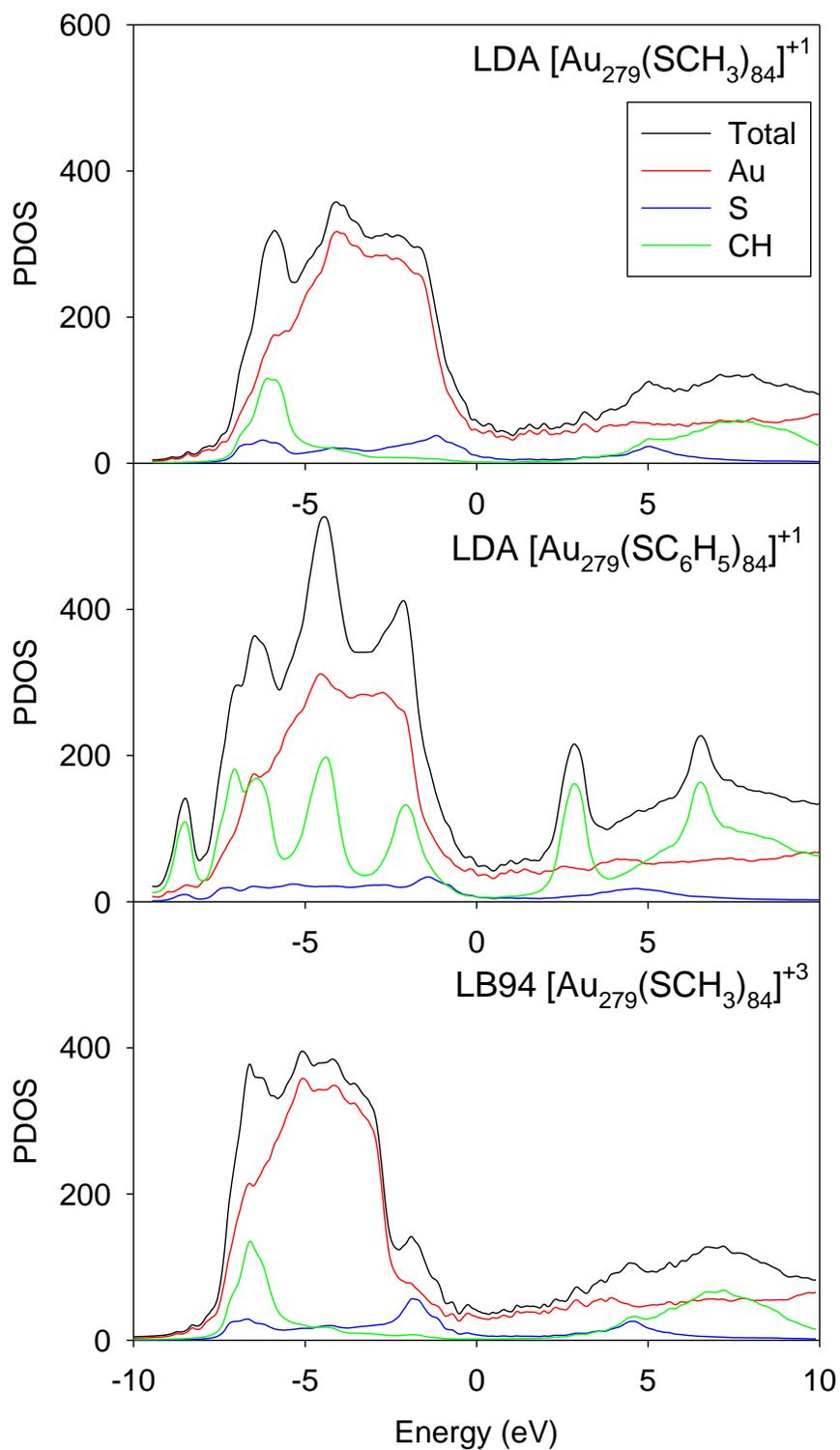
**Table S1. Three major series of Thiolate Protected NMs reported till date with >200 Au atoms.**

PC2S		TBBT		<i>p</i> -MBT	
(Au, SR)	Type	(Au, SR)	Type	(Au, SR)	Type
(25,18)	Molecule-like	(28,20)	Molecule-like	(130,50)	Molecule-like
(38,24)	Molecule-like	(36,24)	Molecule-like	(246,80)	Molecule-like
(67,35)	Molecule-like	(44,28)	Molecule-like		
(~103,~45)	Molecule-like	(52,32)	Molecule-like		
(130,50)	Molecule-like	(92,44)	Molecule-like		
(137,56)	Molecule-like	(133,52)	Molecule-like		
(144,60)	Molecule-like	(279,84)	Metal-like		
(329,84)	Metal-like				
(~500,~120)	Metal-like				
(~940,~160)	Metal-like				

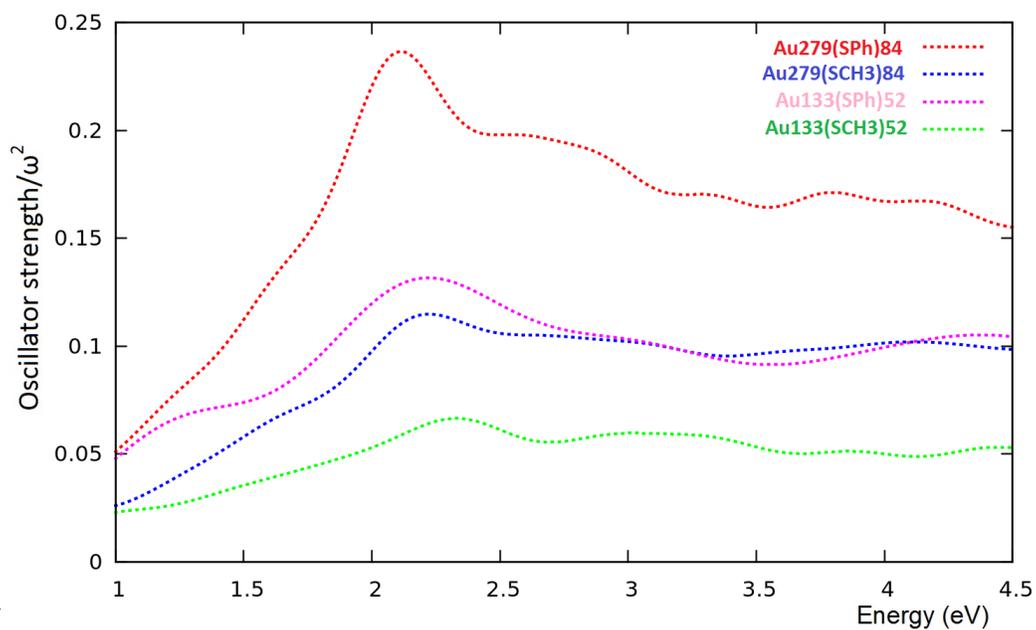
Numbers in the parentheses indicates (number of Au atoms, number of ligands). PC2S – Phenylethane thiolate, TBBT - 4-*tert*-butylbenzene thiolate, and *p*-MBT – 4-methylbenzene thiolate. Sizes indicated in red color are not as stable as other sizes indicated in black fonts.



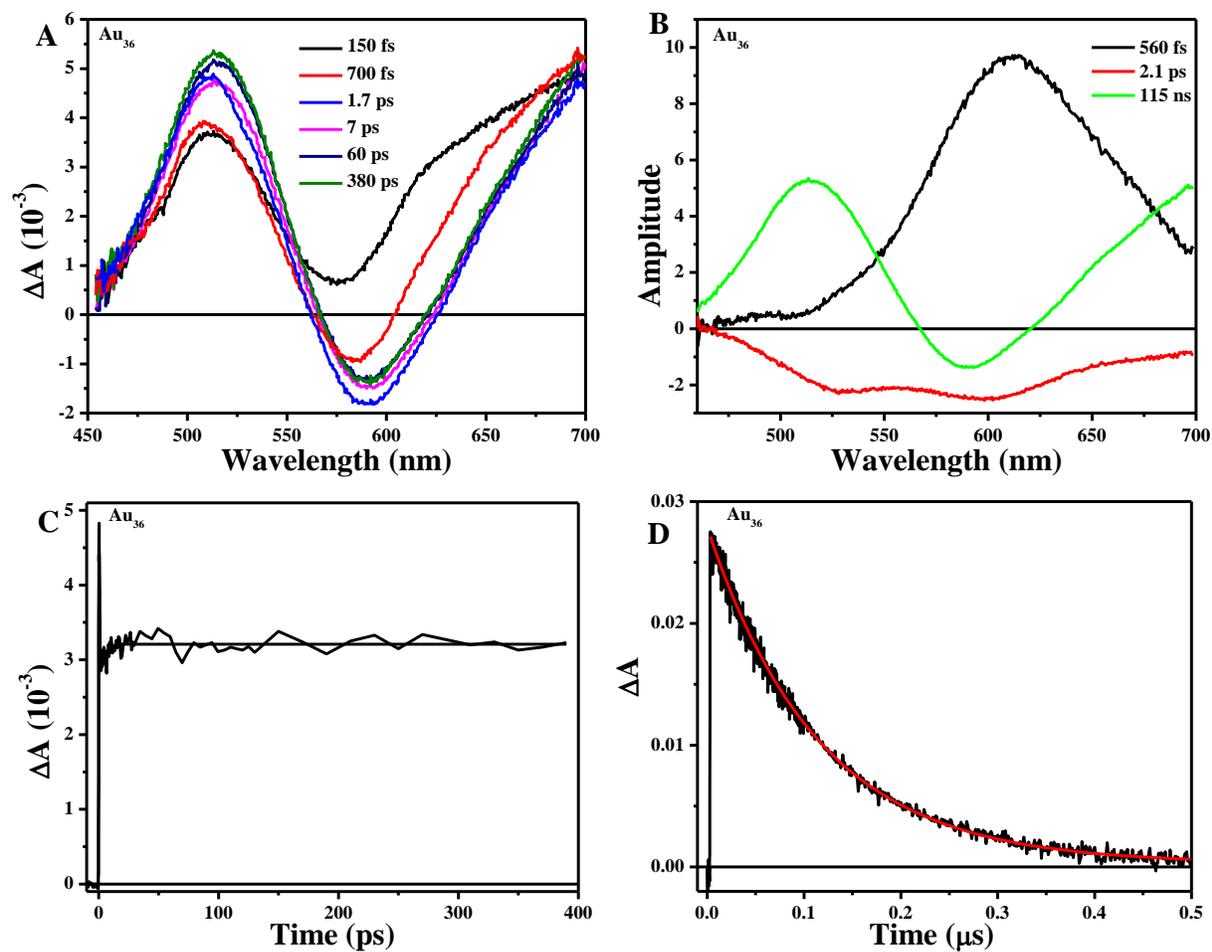
**Figure S1.** Stability of Au<sub>279</sub> and no intermediate stable sizes between Au<sub>133</sub> and Au<sub>279</sub>. “Figure S7. Stability of F-279 nanocrystals under thermochemical treatment for a period of 10 days. \* indicates polydisperse metastable clusters and α indicates polydisperse plasmonic particles.”<sup>4</sup>



**Figure S2.** PDOS of  $[\text{Au}_{279}(\text{SR})_{84}]^{+q}$  systems with two different ligands (R) and xc-functionals ( $q=+1$  for LDA,  $q=+3$  for LB94) with the zero of energy set at the Fermi energy.

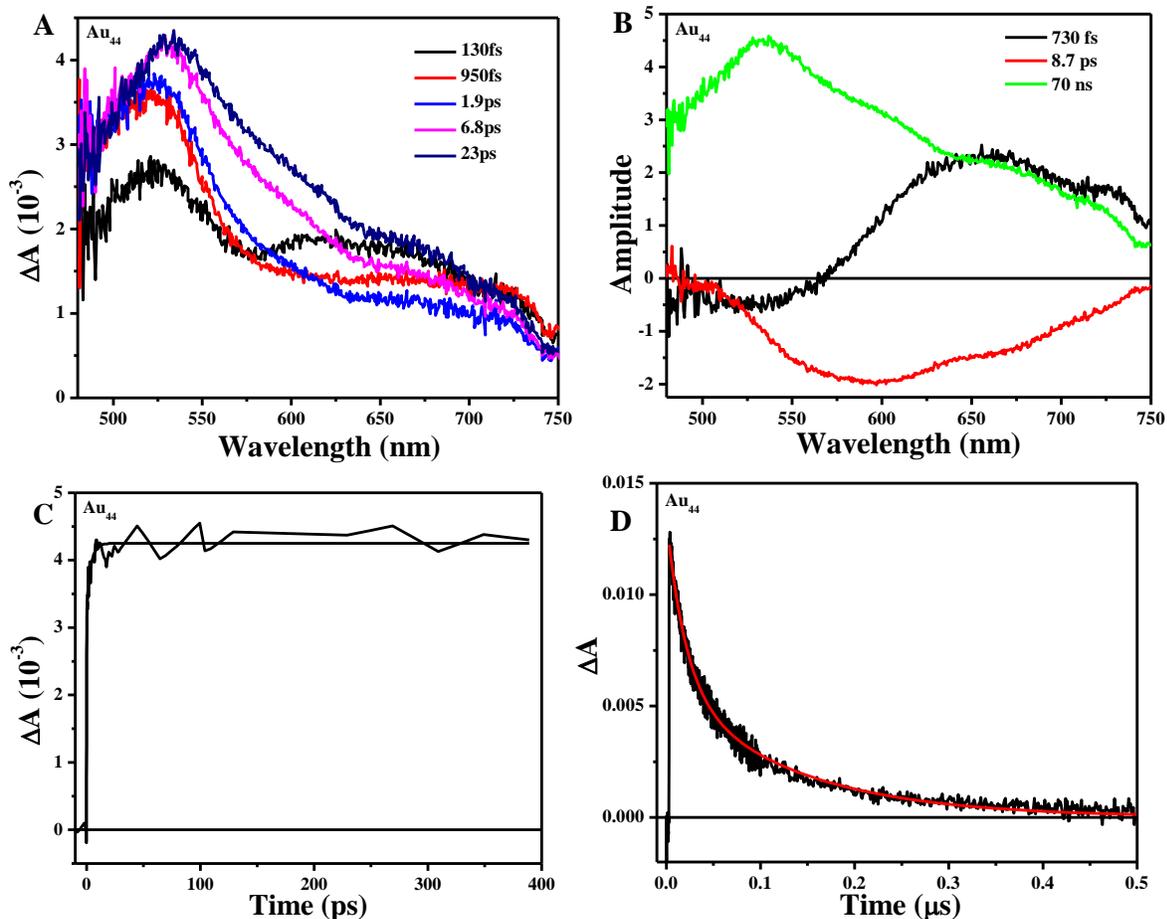


**Figure S3.** RT-TDFT simulated spectra along the z-Cartesian component of the electric field of  $\text{Au}_{279}(\text{SPh})_{84}$ ,  $\text{Au}_{279}(\text{SCH}_3)_{84}$ ,  $\text{Au}_{133}(\text{SPh})_{52}$ ,  $\text{Au}_{133}(\text{SCH}_3)_{52}$ , using the VS98 xc-functional.

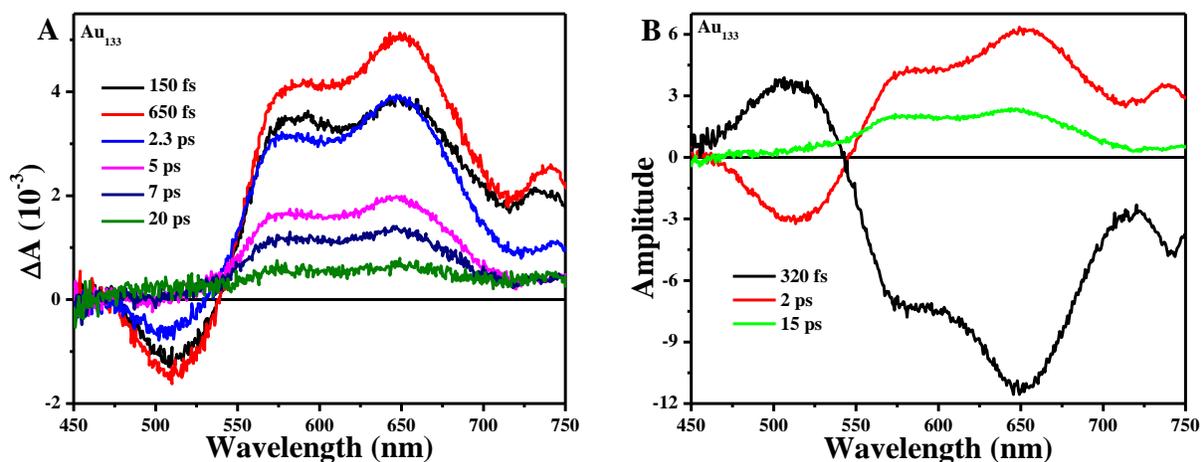


**Figure S4.** (A) Excited state absorption spectra at different time delays, (B) Species associated spectra obtained from global fit analysis and (C) Kinetic decay trace at 660 nm of Au<sub>36</sub> after excitation at 370 nm. (D) Nanosecond decay trace of Au<sub>36</sub> monitored at 660 nm.

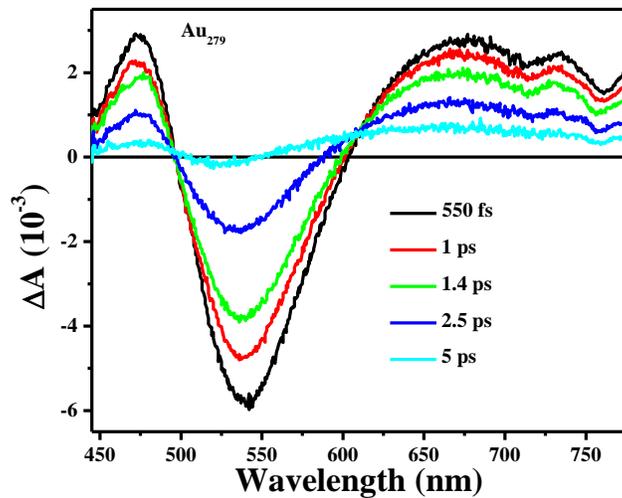




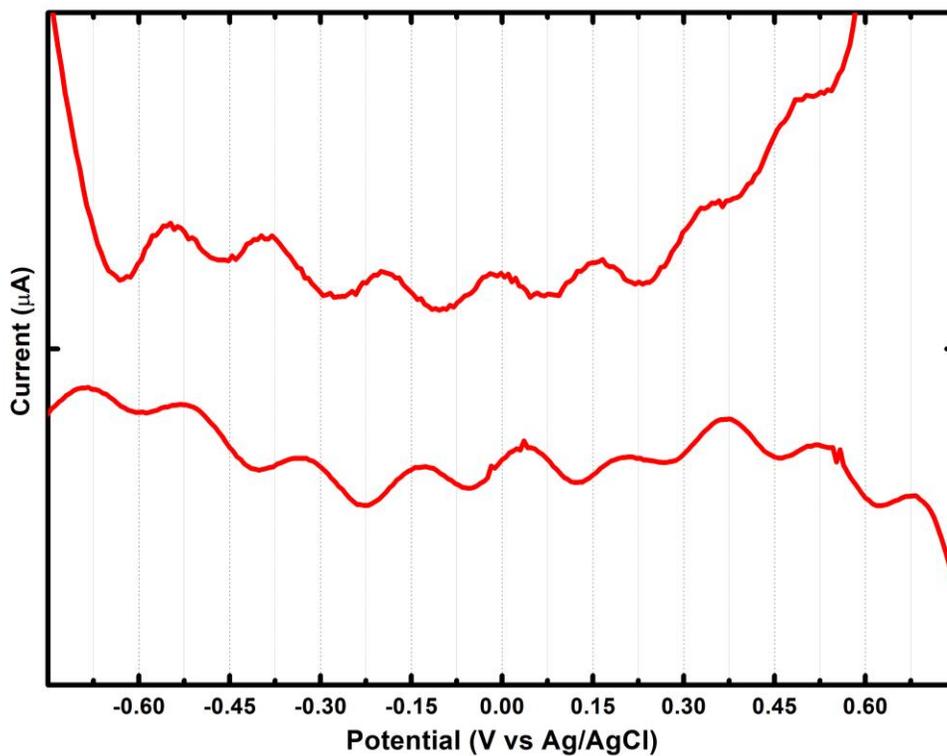
**Figure S5.** (A) Excited state absorption spectra at different time delays, (B) species associated spectra obtained from global fit analysis and (C) Kinetic decay trace at 525 nm of Au<sub>44</sub> after excitation at 370 nm. (D) Nanosecond decay trace of Au<sub>44</sub> monitored at 525 nm.



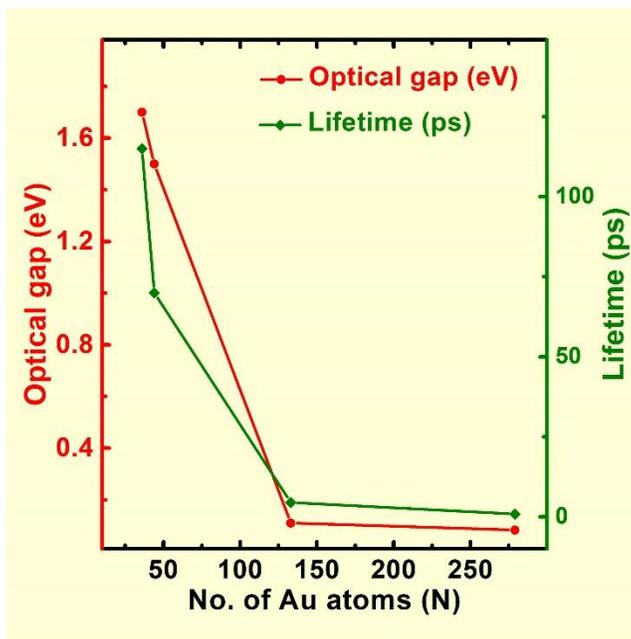
**Figure S6.** (A) Excited state absorption spectra at different time delays, (B) species associated spectra obtained from global fit analysis of Au<sub>133</sub> after excitation at 370 nm.



**Figure S7.** Excited state absorption spectra at different time delays of Au<sub>279</sub> after excitation at 370 nm.



**Figure S8.** Differential pulse voltammetry of Au<sub>279</sub>(SC<sub>10</sub>H<sub>13</sub>)<sub>84</sub>.



**Figure S9.** Size-dependent optical gap and lifetime trend observed for Au<sub>36</sub>, Au<sub>44</sub>, Au<sub>133</sub> and Au<sub>279</sub> TBBT protected nanomolecules. Red line with circles indicates the optical gap and the green line with rhombus indicates the lifetime vs number of gold atoms.

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**Table S2. Cartesian Coordinates of Au<sub>279</sub>(SPh)<sub>84</sub>**

Au	17.5578802755	9.8472687328	9.7220431130
Au	16.3876502755	13.7000487328	5.2374131129
Au	19.0781402755	12.2022887328	8.7734231130
Au	14.3945502755	-0.2418512672	3.5068931130
Au	18.1717002755	4.3703287328	7.1709731129
Au	11.8034202755	7.5835487328	-2.7224768871
Au	2.9320302755	17.4281787328	11.7123831129
Au	13.1266202755	14.9111187328	1.8945131130
Au	9.4597502755	5.7858687328	6.9551331129
Au	10.7893402755	7.7692887328	8.5727931130
Au	12.6734502755	9.5646487328	7.3146531130
Au	8.3491202755	6.1768087328	12.6017931129
Au	7.9213402755	12.2447087328	10.6069931129
Au	11.3797602755	7.5731887328	5.7400031130
Au	6.9868002755	4.1934087328	10.9965831129
Au	11.6858402755	5.7390987328	10.3254931129
Au	6.6541302755	6.0259787328	6.4316331130
Au	5.6961902755	8.0265387328	4.6207831130
Au	12.1283302755	9.7595787328	10.1648731129
Au	4.6398502755	8.5052487328	10.3090031129
Au	10.0028402755	5.5892587328	4.1456731129
Au	8.8430502755	10.1896787328	12.3496931129
Au	8.4455302755	12.0532187328	7.7536131130
Au	10.7102502755	12.0063387328	11.1734931129
Au	5.5324202755	6.4551587328	12.0134231129
Au	7.4661602755	8.2163887328	10.8134631129
Au	6.0994702755	6.2310487328	9.2435931130
Au	4.1932702755	4.4452987328	10.4984531129
Au	10.3332402755	3.7412587328	8.7450731130
Au	9.7484402755	8.1687387328	14.2244731129
Au	7.6172402755	9.7906687328	3.3928931130
Au	5.6577802755	12.2637787328	7.2504231130
Au	11.1908002755	11.7841087328	8.3715031130
Au	7.1910202755	5.8606987328	3.6265731130
Au	6.5619702755	10.2649187328	9.0295031130
Au	11.6450002755	9.9500587328	12.9487131129
Au	4.8019702755	4.2441387328	7.7142131130
Au	10.4220802755	9.5255787328	3.9587331130
Au	8.0896002755	3.7797887328	5.3924831129
Au	6.9200302755	8.4073587328	13.5929231129
Au	5.6746802755	2.1639387328	9.4942131130
Au	6.2204602755	12.0065587328	4.3918431130
Au	8.9759402755	11.8095587328	4.9657231130
Au	9.0844102755	7.5816987328	2.3390431129
Au	13.0728502755	7.6874187328	11.9719331129
Au	3.3151602755	6.4856987328	8.7183031130
Au	11.1392802755	5.8840887328	13.1647131129
Au	6.9816302755	14.3205787328	8.7837531130
Au	11.7382902755	11.5565187328	5.5426631129
Au	6.3552002755	4.3788887328	13.7673731129
Au	3.1936902755	10.7315387328	11.3235931129
Au	7.6965002755	6.3327487328	15.3897331129
Au	6.2638802755	7.8617687328	1.7797531129
Au	1.8070702755	8.7559787328	9.7543731130

Au	11.9270202755	7.2958287328	2.9087031130
Au	8.4758802755	1.8874487328	9.9833631130
Au	7.8578302755	2.1848887328	12.7993631129
Au	9.7503102755	14.0656687328	9.3901331130
Au	6.2163202755	1.9235487328	6.6486931130
Au	13.1668702755	3.4726187328	9.2942331130
Au	7.5087702755	14.0552787328	5.9570731129
Au	9.8799702755	9.7900887328	6.7685931130
Au	4.7678902755	10.0603887328	2.7958631130
Au	13.9948402755	11.6180287328	8.9695831129
Au	4.0501702755	8.6905987328	13.1152731129
Au	2.6961602755	6.7132687328	11.4896631129
Au	4.6264702755	12.6941087328	12.9709431129
Au	8.2583502755	10.3544087328	15.1535931129
Au	5.5303502755	10.6968687328	14.6910031129
Au	10.8806002755	3.5825687328	5.8847131130
Au	9.1122902755	4.0522187328	14.4750931129
Au	5.0399602755	2.3769687328	12.3252231129
Au	13.2858802755	9.3278187328	4.4683331129
Au	4.2069202755	14.4492287328	8.3157331129
Au	10.3197902755	13.8790887328	6.5637531130
Au	9.5187802755	11.5067287328	2.1106231129
Au	12.8705602755	5.3384287328	4.6856931130
Au	13.5603302755	11.8442987328	11.7292731129
Au	14.4547502755	5.5165387328	10.8369231129
Au	2.9022702755	8.2859787328	4.0962931129
Au	2.4909502755	4.2097787328	4.3968031129
Au	10.1939402755	12.1330187328	13.9794231129
Au	12.5387902755	8.0524587328	14.7624331129
Au	6.4912102755	14.4367887328	11.6807831129
Au	6.3870002755	8.6086687328	16.4002531129
Au	3.4274402755	12.2810387328	3.8923331130
Au	1.0349102755	6.3923987328	5.3749531130
Au	14.9242202755	9.5697487328	10.6667131129
Au	7.9930902755	8.0118787328	8.0029131130
Au	4.7414202755	14.2591787328	5.4493231130
Au	1.3310902755	4.6236387328	9.9409631129
Au	11.2321602755	1.7487987328	10.5254631129
Au	14.3647402755	9.6851387328	13.4510631129
Au	2.3355502755	12.7122887328	9.5575731129
Au	1.0038902755	10.6988987328	7.9264031130
Au	13.0764502755	13.5441487328	7.1088531130
Au	12.3274602755	11.3149687328	2.7747731130
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H	19.0512907220	4.4919235163	2.4680430405
H	14.0220932886	-3.1425373068	2.4502882163
H	15.0787216413	-5.1375437397	1.3315613842
H	15.4790424578	-5.1301229097	-1.1738841997
H	14.8227317995	-3.1025184998	-2.5381359223
H	13.8285961363	-1.0905825592	-1.4041855576
H	0.8711610875	13.2082218515	15.1588053914
H	-0.6575130862	12.5966285563	17.0867026686
H	-2.9836327259	13.5740130693	17.2056868779
H	-3.7950924314	15.1327718474	15.3928281667
H	-2.2878493584	15.7042200161	13.4468236167
H	17.6091509039	4.2338407944	14.6144763488
H	18.9486919757	3.2869884935	16.5403461225
H	18.9304148661	4.4517797279	18.7912057789
H	17.6297938556	6.5901554155	19.0949371606
H	16.3297174585	7.5581197751	17.1487794683
H	3.4982073353	9.4281130908	-1.6209884359
H	1.5795205977	8.8654077587	-3.1736581989
H	1.3850293694	10.0464951865	-5.4087865484
H	3.0451895684	11.8600656097	-6.0220485276
H	4.8889199474	12.4929879579	-4.4131401063
H	-0.3701069011	10.3411383841	-1.1231032641
H	-2.0523104972	11.5987680698	-2.5295523506
H	-1.8421199608	14.1028473450	-2.8023319084

H	0.0537261761	15.3437882464	-1.6609565229
H	1.8022646380	14.0610342125	-0.3408556057
H	10.3009747420	-3.5972057961	7.5736905474
H	9.0172625052	-5.7617756962	7.5349982851
H	8.9773816831	-7.1680426663	5.4160416480
H	10.2368763692	-6.3952885053	3.3797240975
H	11.5393359335	-4.2274422690	3.4268022909
H	-1.3682813588	16.4581906285	9.9686556686
H	-3.5182411647	17.3124683437	11.0087414783
H	-3.5227055973	19.4790667554	12.3295877750
H	-1.3579470918	20.7237927794	12.6890438692
H	0.8046620077	19.8187905114	11.7272934990
H	-2.3655278490	5.0837096534	15.8744262819
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H	6.5743263579	-1.5791165484	-0.5483745324
H	7.9059593293	-2.9511460847	-2.2393409012
H	8.8687993367	-1.8500618779	-4.2845761704
H	8.4532782325	0.6229561837	-4.7009805543
H	7.1493892639	1.9781838692	-3.0305720925
H	7.8788297703	11.8305565819	-4.1202883988
H	6.4490374307	12.3271194700	-6.1566740376
H	5.9951008185	14.7218940007	-6.8400195620
H	6.9816202204	16.6217560065	-5.5055584476
H	8.4356209880	16.1202613501	-3.4773018280
H	5.3787420648	3.7455255177	-1.8062645123
H	4.9934393297	1.9089111941	-3.5113903889
H	4.0970156342	2.4771148520	-5.8052250822
H	3.5822549384	4.8759594012	-6.3968556481
H	3.9631919061	6.7093332208	-4.6888207072
H	5.4906874600	16.7284843310	-3.6481150795
H	5.9706404690	19.1651043907	-4.1257959649
H	6.7112154894	20.7029554746	-2.2742284674
H	6.8443784148	19.8346507642	0.1016217638
H	6.3685702085	17.3997839436	0.5833767819
H	9.2747935218	19.0349258958	10.0141391504
H	9.5127373497	21.4564554080	9.2783346731
H	8.0844997329	23.2475937863	10.3519187016
H	6.4607544191	22.6382959709	12.1814022781
H	6.2688566446	20.2306025756	12.9526677067
H	-3.9790560707	4.0388208127	12.1706971982
H	-5.8950298284	4.5680253724	13.7612656060
H	-6.0543749141	3.3562615839	15.9756523826
H	-4.3383805135	1.6037540933	16.5817359846
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H	11.7230978480	17.8552359283	5.4233012502
H	13.3064399936	19.8124343926	5.5195277294
H	12.4698863760	22.1036305739	6.2369032518
H	10.0223788497	22.4154371835	6.7944344675
H	8.4347369028	20.4436674354	6.6727443103
H	12.7841131481	3.8334492185	-5.7007463198
H	14.9980944669	3.8450213843	-6.9135128571
H	16.9317690550	5.2159414890	-6.0243518828
H	16.6434675146	6.5847148997	-3.9279050060
H	14.4224376988	6.5823920140	-2.7119424541

H	2.6473298772	5.3069382962	-0.7913777385
H	1.8214088236	3.7180617808	-2.5676696090
H	-0.5197441162	3.9454451483	-3.5059474329
H	-1.9963187705	5.8497821264	-2.7060067619
H	-1.1550557540	7.4518124144	-0.9501585954
H	10.8686138710	-1.6619511199	-2.3790548199
H	12.7015346955	-2.3566880519	-3.9761902120
H	14.4746579906	-0.6778107971	-4.6731850482
H	14.4251912188	1.6614108323	-3.7326843337
H	12.5685559766	2.3683779609	-2.1642923416
H	0.6165119927	-2.5587231701	15.7422213351
H	0.7885577153	-5.0736936261	16.0217404986
H	2.1427298107	-6.4364682689	14.3974737779
H	3.3602900235	-5.2904231874	12.4791157259
H	3.2222170214	-2.7756435606	12.2437403756
H	15.9308404203	-2.3743672661	12.9184313214
H	17.3759989109	-3.8181216690	14.4053302051
H	16.7271154925	-4.1975346268	16.8193024728
H	14.7145425409	-2.9973819252	17.7817863510
H	13.2677525765	-1.5381554072	16.2768813858
H	13.5331158463	19.4285250722	15.6712235447
H	14.0162008094	21.9127061817	15.5080021357
H	12.6722078148	23.3484420093	13.9157547833
H	10.8301153802	22.3172978527	12.5235498700
H	10.3562488160	19.8229416052	12.7061125352
H	15.8116887828	12.3663949617	0.6467157363
H	15.9469200994	13.8558166222	-1.4034277374
H	17.2609128279	16.0078921635	-1.3200800062
H	18.4928166762	16.6491111517	0.8112798085
H	18.2850377711	15.2022388418	2.8635328773
H	10.9689218553	-3.0811629485	16.2643824640
H	12.0815505111	-3.9758900826	18.3461236441
H	11.8095719532	-2.7512102323	20.5478254288
H	10.4249247129	-0.6457610931	20.6514184490
H	9.2867823609	0.2418476089	18.5556601405
H	-1.1572902521	14.9995425114	0.5352099728
H	-2.8463415255	16.8868136152	0.5750408599
H	-4.0118737901	17.4987235373	2.7293275977
H	-3.5189966731	16.2057305200	4.8460811387
H	-1.7940301128	14.3455170570	4.8085918508
H	-2.4719698721	12.4649412921	12.4607391983
H	-4.5726887083	13.8905711351	12.4601829226
H	-6.4914514762	13.3021050204	10.9260989372
H	-6.2839723866	11.3295210370	9.3460940459
H	-4.1424810179	9.9907240759	9.2669385875
H	20.0230395911	2.0989219257	10.4323276928
H	21.9993711180	1.4321838286	9.0184166357
H	23.4414075651	3.2083049475	7.9349242338
H	22.8864585059	5.6450547792	8.2592539909
H	20.9097943621	6.3164067961	9.6943255146
H	17.0689953227	7.6854890636	-1.7129080124
H	18.2345391931	9.3711319165	-3.2079982764
H	17.2162889788	11.6407875135	-3.5927156754
H	15.0510093415	12.2558596349	-2.4542848793
H	13.9287945156	10.6088737380	-0.8787896171
H	5.6129142431	9.8313141836	20.1842792630
H	5.6953957851	8.3963705595	22.2481092039



H	3.8981977503	6.6446703055	22.6511963311
H	2.0433155997	6.3464483369	20.9670821239
H	1.9310883756	7.8271442720	18.9233845305
H	21.7494103430	7.7710437220	10.7521173679
H	24.0879194624	8.5478083522	10.1410163730
H	24.5832589973	11.0167928619	9.8975095465
H	22.7709374177	12.7143122780	10.3522964829
H	20.4486263019	11.9323935229	10.9943649091
H	3.8690029371	2.2338755313	18.3308136219
H	3.7904866194	0.6287849896	20.2845284822
H	4.3040190068	1.4528484852	22.6132018996
H	4.9059741199	3.8968877771	22.9882502589
H	5.0559933682	5.4673743659	20.9996657841
H	18.9309659044	8.7133506879	14.4266514868
H	19.8476982755	8.1958944149	16.7293675815
H	18.7564271724	9.1997984925	18.7753270550
H	16.7230804905	10.6851913112	18.5224584454
H	15.8048983709	11.1818220347	16.2248996539
H	6.8923656530	2.5809457105	-5.2072181146
H	7.4928718535	1.7980254532	-7.5189304266
H	9.6625273823	2.5522248680	-8.5930389708
H	11.1864422181	4.1448473859	-7.3543393420
H	10.5508908281	4.9669425382	-5.0537937865
H	2.3939625004	20.5605313799	6.4458969239
H	0.4878320577	22.0324561814	5.6613734459
H	-1.6864231757	20.9888376213	4.9097541097
H	-1.9802495353	18.4835925688	4.9912947000
H	-0.0729439112	17.0086161052	5.7927391948
H	-2.4690483350	10.6257448295	14.7895521184
H	-3.7388219809	9.7549797634	16.8030697265
H	-2.5026059362	8.5021100524	18.6215398356
H	-0.0163054139	8.1152144785	18.4202088593
H	1.2539294663	8.9999709109	16.4191949173
H	-4.0784671794	14.1521741197	5.5287683014
H	-5.7542086004	14.8265897769	3.7523664048
H	-6.9509130617	13.0582285599	2.4146729335
H	-6.4827435789	10.6090977062	2.8420416859
H	-4.8099775968	9.9450484458	4.6481432250
H	6.7658241606	-3.4049804921	2.9915897712
H	4.9593155881	-4.8473783663	1.9571386366
H	5.1979907770	-5.6553491217	-0.4125920194
H	7.3205983534	-5.1349095901	-1.7188406374
H	9.1041839338	-3.6615641152	-0.6751505504
H	-2.8974267338	6.5827155084	2.3013162243
H	-3.6447330722	5.6647019420	0.0563813153
H	-3.7353786920	7.1899838926	-1.9522575248
H	-3.1932722966	9.6504488872	-1.7064197221
H	-2.4535682552	10.5608062086	0.5546518191
H	5.5306523035	-2.7827829754	11.0667447691
H	5.4817925347	-5.3055231537	10.9021064915
H	6.4189694986	-6.7196602660	12.7768522529
H	7.4054485187	-5.6086141606	14.8216027248
H	7.4198424563	-3.0966855328	15.0040334855
H	-1.0516534790	0.6314599276	16.0949081625
H	-1.4711443637	-1.4622062918	17.4427255480
H	0.4358180310	-2.5462983715	18.7174105830
H	2.7069200572	-1.4563478342	18.7367064991

H	3.1318435785	0.6253482970	17.3807290404
H	-0.6652573442	-1.2710603146	7.1488916643
H	-3.1096352167	-1.7832960120	7.4760498265
H	-4.8286715546	-0.8496812423	5.8506493336
H	-4.0736888798	0.6625419051	3.9674501663
H	-1.6176989307	1.1218563640	3.6182445666
H	-2.9066370993	0.9987031245	9.1473600509
H	-5.1886750662	0.7212028201	10.2004972068
H	-5.4934449963	-0.8306937799	12.1883464110
H	-3.5365876430	-2.1923783219	13.0240547930
H	-1.2589397226	-1.9426853593	11.9292768758
H	9.2209679186	19.7009041791	-1.1247277976
H	10.5164614751	21.8729041160	-0.9556652217
H	12.4174725462	22.0855056585	0.7108596577
H	13.1181184236	20.0806758237	2.0609484258
H	11.8244473900	17.9172437446	1.8964314801
H	13.5507130202	-4.1665068554	11.0495939668
H	15.6067047073	-5.5941475619	11.4989426248
H	17.9018924705	-4.6943293772	10.9655022292
H	18.1625307522	-2.3747239449	9.9811319041
H	16.0863605339	-0.9695038971	9.5145796099
H	2.7877178316	-2.3181368708	4.9143287579
H	0.4053494074	-3.0848000505	4.4275134116
H	-0.4160902318	-3.2110494873	2.0468530636
H	1.1197613688	-2.5481899495	0.1366026587
H	3.4812563763	-1.7546867589	0.6443162650
H	14.1064526739	17.6078153754	7.9666287930
H	16.3455787927	18.7595115549	8.2799644711
H	16.7015125914	20.3083222075	10.2338588134
H	14.7904047004	20.8333193681	11.7997005945
H	12.5411625991	19.7296462000	11.4679013443
H	-4.6520278645	8.0043897791	10.2425645892
H	-5.7815208202	9.2360177362	12.1495237322
H	-4.8879086293	9.0041541351	14.5092389077
H	-2.9627589435	7.4128770578	14.9786608480
H	-1.9422129276	6.1011964553	13.0925146282

**Table S3. Cartesian Coordinates of Au<sub>279</sub>(SCH<sub>3</sub>)<sub>84</sub>**

Au	17.5578802755	9.8472687328	9.7220431130
Au	16.3876502755	13.7000487328	5.2374131129
Au	19.0781402755	12.2022887328	8.7734231130
Au	14.3945502755	-0.2418512672	3.5068931130
Au	18.1717002755	4.3703287328	7.1709731129
Au	11.8034202755	7.5835487328	-2.7224768871
Au	2.9320302755	17.4281787328	11.7123831129
Au	13.1266202755	14.9111187328	1.8945131130
Au	9.4597502755	5.7858687328	6.9551331129
Au	10.7893402755	7.7692887328	8.5727931130
Au	12.6734502755	9.5646487328	7.3146531130
Au	8.3491202755	6.1768087328	12.6017931129
Au	7.9213402755	12.2447087328	10.6069931129
Au	11.3797602755	7.5731887328	5.7400031130
Au	6.9868002755	4.1934087328	10.9965831129
Au	11.6858402755	5.7390987328	10.3254931129
Au	6.6541302755	6.0259787328	6.4316331130
Au	5.6961902755	8.0265387328	4.6207831130
Au	12.1283302755	9.7595787328	10.1648731129
Au	4.6398502755	8.5052487328	10.3090031129
Au	10.0028402755	5.5892587328	4.1456731129
Au	8.8430502755	10.1896787328	12.3496931129
Au	8.4455302755	12.0532187328	7.7536131130
Au	10.7102502755	12.0063387328	11.1734931129
Au	5.5324202755	6.4551587328	12.0134231129
Au	7.4661602755	8.2163887328	10.8134631129
Au	6.0994702755	6.2310487328	9.2435931130
Au	4.1932702755	4.4452987328	10.4984531129
Au	10.3332402755	3.7412587328	8.7450731130
Au	9.7484402755	8.1687387328	14.2244731129
Au	7.6172402755	9.7906687328	3.3928931130
Au	5.6577802755	12.2637787328	7.2504231130
Au	11.1908002755	11.7841087328	8.3715031130
Au	7.1910202755	5.8606987328	3.6265731130
Au	6.5619702755	10.2649187328	9.0295031130
Au	11.6450002755	9.9500587328	12.9487131129
Au	4.8019702755	4.2441387328	7.7142131130
Au	10.4220802755	9.5255787328	3.9587331130
Au	8.0896002755	3.7797887328	5.3924831129
Au	6.9200302755	8.4073587328	13.5929231129
Au	5.6746802755	2.1639387328	9.4942131130
Au	6.2204602755	12.0065587328	4.3918431130
Au	8.9759402755	11.8095587328	4.9657231130
Au	9.0844102755	7.5816987328	2.3390431129
Au	13.0728502755	7.6874187328	11.9719331129
Au	3.3151602755	6.4856987328	8.7183031130
Au	11.1392802755	5.8840887328	13.1647131129
Au	6.9816302755	14.3205787328	8.7837531130
Au	11.7382902755	11.5565187328	5.5426631129
Au	6.3552002755	4.3788887328	13.7673731129
Au	3.1936902755	10.7315387328	11.3235931129
Au	7.6965002755	6.3327487328	15.3897331129
Au	6.2638802755	7.8617687328	1.7797531129
Au	1.8070702755	8.7559787328	9.7543731130

Au	11.9270202755	7.2958287328	2.9087031130
Au	8.4758802755	1.8874487328	9.9833631130
Au	7.8578302755	2.1848887328	12.7993631129
Au	9.7503102755	14.0656687328	9.3901331130
Au	6.2163202755	1.9235487328	6.6486931130
Au	13.1668702755	3.4726187328	9.2942331130
Au	7.5087702755	14.0552787328	5.9570731129
Au	9.8799702755	9.7900887328	6.7685931130
Au	4.7678902755	10.0603887328	2.7958631130
Au	13.9948402755	11.6180287328	8.9695831129
Au	4.0501702755	8.6905987328	13.1152731129
Au	2.6961602755	6.7132687328	11.4896631129
Au	4.6264702755	12.6941087328	12.9709431129
Au	8.2583502755	10.3544087328	15.1535931129
Au	5.5303502755	10.6968687328	14.6910031129
Au	10.8806002755	3.5825687328	5.8847131130
Au	9.1122902755	4.0522187328	14.4750931129
Au	5.0399602755	2.3769687328	12.3252231129
Au	13.2858802755	9.3278187328	4.4683331129
Au	4.2069202755	14.4492287328	8.3157331129
Au	10.3197902755	13.8790887328	6.5637531130
Au	9.5187802755	11.5067287328	2.1106231129
Au	12.8705602755	5.3384287328	4.6856931130
Au	13.5603302755	11.8442987328	11.7292731129
Au	14.4547502755	5.5165387328	10.8369231129
Au	2.9022702755	8.2859787328	4.0962931129
Au	2.4909502755	4.2097787328	4.3968031129
Au	10.1939402755	12.1330187328	13.9794231129
Au	12.5387902755	8.0524587328	14.7624331129
Au	6.4912102755	14.4367887328	11.6807831129
Au	6.3870002755	8.6086687328	16.4002531129
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C	17.0510640259	5.5582667687	15.1167572462
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