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Unraveling a generic growth pattern in structure evolution of thiolate-protected gold nanoclusters†

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Precise control of the growth of thiolate-protected gold nanoclusters is a prerequisite for their applications in catalysis and bio-engineering. Here, we bring to bear a new series of thiolate-protected nanoclusters with a unique growth pattern, *i.e.*, Au₂₀(SR)₁₆, Au₂₈(SR)₂₀, Au₃₆(SR)₂₄, Au₄₄(SR)₂₈, and Au₅₂(SR)₃₂. These nanoclusters can be viewed as resulting from the stepwise addition of a common structural motif [Au₈(SR)₄]. The highly negative values of the nucleus-independent chemical shift (NICS) in the center of the tetrahedral Au₄ units suggest that the overall stabilities of these clusters stem from the local stability of each tetrahedral Au₄ unit. Generalization of this growth-pattern rule to large-sized nanoclusters allows us to identify the structures of three new thiolate-protected nanoclusters, namely, Au₆₀(SR)₃₆, Au₆₈(SR)₄₀, and Au₇₆(SR)₄₄. Remarkably, all three large-sized nanoclusters possess relatively large HOMO–LUMO gaps and negative NICS values, suggesting their high chemical stability. Further extension of the growth-pattern rule to the infinitely long nanowire limit results in a one-dimensional (1D) thiolate-protected gold nanowire (RS–AuNW) with a band gap of 0.78 eV. Such a unique growth-pattern rule offers a guide for precise synthesis of a new class of large-sized thiolate-protected gold nanoclusters or even RS–AuNW which, to our knowledge, has not been reported in the literature.

Introduction

Since the first successful crystallization of the thiolate-protected gold nanocluster Au₁₀₂(SR)₄₄ in 2007,¹ research into

the structural evolution and structure–property relationship of thiolate-protected gold nanoclusters has attracted considerable attention due to high potential of these nanoclusters for applications in electronics, catalysis and bioengineering.^{2–7} Significant advancement in structure determination has been made on the basis of X-ray crystallography,^{1,8–20} single-particle transmission electron microscopy (SP-TEM),²¹ as well as density-functional theory (DFT) computation^{22–30} in conjunction with the “divide and protect” formulation.^{4,31} Although the latter formulation can be very useful in seeking optimal ligand patterns for given gold-core structures, generic growth patterns of the gold nanoclusters are still largely unknown, which hinders the development of large-sized ligand-protected gold nanoclusters for optical and electronic applications.

In this communication, we report a growth-pattern rule that has been revealed based on previously known (*via* X-ray crystallography) and/or theoretically predicted structures of a series of ligand-protected gold nanoclusters, *i.e.*, Au₂₀(SR)₁₆,^{25,32} Au₂₈(SR)₂₀,^{13,40} Au₃₆(SR)₂₄,¹⁵ Au₄₄(SR)₂₈,^{28,33} and Au₅₂(SR)₃₂.¹² These clusters can be viewed as structural evolutions from the starting cluster Au₂₀(SR)₁₆ *via* sequential addition of a [Au₈(SR)₄] motif, *i.e.*, Au₂₀(SR)₁₆ + [Au₈(SR)₄] → Au₂₈(SR)₂₀ + [Au₈(SR)₄] → Au₃₆(SR)₂₄ + [Au₈(SR)₄] → Au₄₄(SR)₂₈ + [Au₈(SR)₄] → Au₅₂(SR)₃₂. Fig. 1 illustrates the structural evolution of the face-centered-cubic (FCC) type of Au kernels in these clusters *via* sequential addition of the “boat-like” Au₈ motif.

Computational methods

All clusters were optimized using the DFT method implemented in the Dmol³ 7.0 code.^{34,35} To this end, the generalized gradient approximation in the Perdew–Burke–Ernzerhof (PBE)³⁶ form was employed together with the double numeric polarized (DNP) basis set and the semi-core pseudopotential. In all our computations, the R group in the ligands is simplified as a methyl group or hydrogen atom. All the optimized structures of the nanoclusters are presented in ESI Fig. S1.† On basis of the optimized structures (R = hydro-

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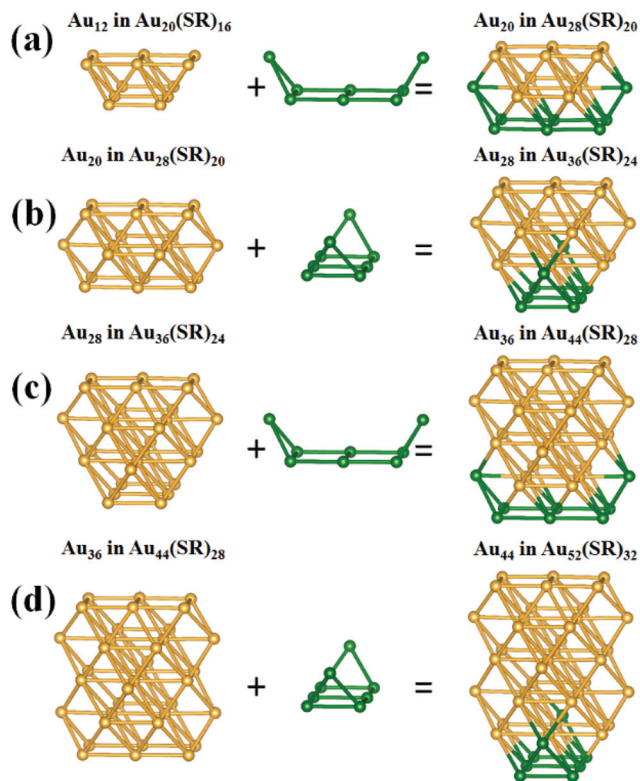


Fig. 1 Au-kernel growth by adding the "boat-like" Au_8 motif (olive). (a) Au_{12} in $\text{Au}_{20}(\text{SR})_{16}$ to Au_{20} in $\text{Au}_{28}(\text{SR})_{20}$. (b) Au_{20} in $\text{Au}_{28}(\text{SR})_{20}$ to Au_{28} in $\text{Au}_{36}(\text{SR})_{24}$. (c) Au_{28} in $\text{Au}_{36}(\text{SR})_{24}$ to Au_{36} in $\text{Au}_{44}(\text{SR})_{28}$. (d) Au_{36} in $\text{Au}_{44}(\text{SR})_{28}$ to Au_{44} in $\text{Au}_{52}(\text{SR})_{32}$. According to the deduction of Zeng *et al.*,³³ the structures of these nanoclusters can be characterized as $\text{Au}_{12}[\text{Au}_2(\text{SR})_3]_4(\text{SR})_4$, $\text{Au}_{20}[\text{Au}_2(\text{SR})_3]_4(\text{SR})_8/\text{Au}_{20}[\text{Au}(\text{SR})_2]_2[\text{Au}_2(\text{SR})_3]_2(\text{SR})_8$, $\text{Au}_{28}[\text{Au}_2(\text{SR})_3]_4(\text{SR})_{12}$, $\text{Au}_{36}[\text{Au}_2(\text{SR})_3]_4(\text{SR})_{16}$, and $\text{Au}_{44}[\text{Au}_2(\text{SR})_3]_4(\text{SR})_{20}$, respectively. Next, the Au-kernels can be derived by removing the $[\text{Au}_2(\text{SR})_3]$ staple motifs and the bridging thiolates ($-\text{SR}-$).

gen atom), nucleus-independent chemical shift (NICS) analysis was performed to examine the aromaticity of the clusters using the B3LYP functional^{37,38} with LANL2DZ and 6-31G* basis set implemented in the Gaussian 09 package.³⁹

Results and discussion

As shown in Table 1, the atomic structures of $\text{Au}_{28}(\text{SR})_{20}$,¹³ $\text{Au}_{36}(\text{SR})_{24}$,¹⁵ and $\text{Au}_{52}(\text{SR})_{32}$ ²⁰ nanoclusters have been determined *via* X-ray crystallography. Note that $\text{Au}_{20}(\text{SR})_{16}$ may have two isomeric structures. The theoretically predicted structure²⁵ (see Fig. 1(a)) can well reproduce the optical absorption spectrum of $\text{Au}_{20}(\text{PET})_{16}$ ($\text{PET} = \text{SCH}_2\text{CH}_2\text{Ph}$),³³ and it has a distinct Au kernel of the crystallized $\text{Au}_{20}(\text{TBBT})_{16}$ ($\text{TBBT} = \text{SPh-}t\text{-Bu}$) cluster.⁸ However, considering the close total energy of these two structures (their energy difference is 0.3 eV with capped methyl groups for simplicity), one of the two isomers is likely the same as the theoretically predicted structure. A similar situation was reported in the cases of $\text{Au}_{40}(o\text{-}$

Table 1 A summary of literature results for a series of ligand-protected gold nanoclusters from $\text{Au}_{20}(\text{SR})_{16}$ to $\text{Au}_{76}(\text{SR})_{44}$. \checkmark : structure determined from X-ray crystallography; p: theoretical prediction; \: synthesized clusters without crystallization; ?: structure unknown; ‡: difference in crystallization, prediction not yet confirmed

| | Experiment | Theory |
|----------------------------------|-------------------------------|------------------------|
| $\text{Au}_{20}(\text{SR})_{16}$ | ‡ (ref. 8 and 32) | p (ref. 25) |
| $\text{Au}_{28}(\text{SR})_{20}$ | \checkmark (ref. 13 and 40) | \checkmark (ref. 41) |
| $\text{Au}_{36}(\text{SR})_{24}$ | \checkmark (ref. 15) | \checkmark (ref. 9) |
| $\text{Au}_{44}(\text{SR})_{28}$ | \ (ref. 33) | p (ref. 28 and 42) |
| $\text{Au}_{52}(\text{SR})_{32}$ | \checkmark (ref. 20) | ? |
| $\text{Au}_{60}(\text{SR})_{36}$ | ? | This work |
| $\text{Au}_{68}(\text{SR})_{40}$ | ? | This work |
| $\text{Au}_{76}(\text{SR})_{44}$ | \ (ref. 43) | This work |

$\text{MBT})_{24}$ ⁴³ ($o\text{-MBT} = \text{ortho-methylbenzenethiol}$) and $\text{Au}_{40}(\text{PET})_{24}$.⁴⁴ The structure prediction of $\text{Au}_{44}(\text{SR})_{28}$ ^{28,33} was based on the structural rules derived from the crystallization of $\text{Au}_{28}(\text{SR})_{20}$ and $\text{Au}_{36}(\text{SR})_{24}$, *i.e.*, $\text{Au}_{28}(\text{SR})_{20} + [\text{Au}_8(\text{SR})_4] \rightarrow \text{Au}_{36}(\text{SR})_{24}$ (Fig. 1(b)) + $[\text{Au}_8(\text{SR})_4] \rightarrow \text{Au}_{44}(\text{SR})_{28}$ (Fig. 1(c)). The excellent agreement between experimental and computed optical absorption spectra of $\text{Au}_{44}(\text{SR})_{28}$ validates the predicted structure of $\text{Au}_{44}(\text{SR})_{28}$, which is solely based on the growth-pattern rule derived from $\text{Au}_{28}(\text{SR})_{20}$ and $\text{Au}_{36}(\text{SR})_{24}$. Additional evidence comes from the crystallization of the $\text{Au}_{52}(\text{SR})_{32}$ nanocluster,²⁰ whose structure can be viewed as adding the $[\text{Au}_8(\text{SR})_4]$ motif to the predicted structure of $\text{Au}_{44}(\text{SR})_{28}$ (Fig. 1(d)). It should be noted that the recently reported $\text{Au}_{28}(\text{S-c-C}_6\text{H}_{11})_{20}$ (where $-\text{c-C}_6\text{H}_{11} = \text{cyclohexyl}$)⁴⁰ cluster exhibits a similar Au_{20} kernel structure to crystallized $\text{Au}_{28}(\text{TBBT})_{20}$ (ESI Fig. S2†). Therefore, the two crystallized structures of $\text{Au}_{28}(\text{SR})_{20}$ can be evolved from $\text{Au}_{20}(\text{SR})_{16}$ (Fig. 1(a)). Besides the different surface-protecting ligands, the two isomeric structures have different staple motifs.

According to the "divide and protect" formulation,⁴⁵ $\text{Au}_{20}(\text{SR})_{16}$, $\text{Au}_{28}(\text{SR})_{20}$, $\text{Au}_{36}(\text{SR})_{24}$, $\text{Au}_{44}(\text{SR})_{28}$, and $\text{Au}_{52}(\text{SR})_{32}$ can be divided into $\text{Au}_8[\text{Au}_3(\text{SR})_4]_4$, $\text{Au}_{14}[\text{Au}_2(\text{SR})_3]_4[\text{Au}_3(\text{SR})_4]_2/\text{Au}_{14}[\text{Au}(\text{SR})_2]_2[\text{Au}_2(\text{SR})_3]_4$, $\text{Au}_{20}[\text{Au}_2(\text{SR})_3]_8$, $\text{Au}_{26}[\text{Au}(\text{SR})_2]_2[\text{Au}_2(\text{SR})_3]_8$, and $\text{Au}_{32}[\text{Au}(\text{SR})_2]_4[\text{Au}_2(\text{SR})_3]_8$, respectively. The Au_8 in $\text{Au}_{20}(\text{SR})_{16}$, Au_{14} in $\text{Au}_{28}(\text{SR})_{20}$, Au_{20} in $\text{Au}_{36}(\text{SR})_{24}$, Au_{26} in $\text{Au}_{44}(\text{SR})_{28}$, and Au_{32} in $\text{Au}_{52}(\text{SR})_{32}$, which are comprised of tetrahedral Au_4 units, can be derived by removing the $[\text{Au}(\text{SR})_2]$, $[\text{Au}_2(\text{SR})_3]$, and $[\text{Au}_3(\text{SR})_4]$ staple motifs, as shown in Fig. 2. It is known that NICS values have been commonly used as an index to measure the local aromaticity of fullerene cages⁴⁶ or small metal clusters.⁴⁷ In addition, NICS analyses have been applied successfully to evaluate the stabilities of gold fullerene structures, such as Au_{32} ⁴⁸ and Au_{42} .⁴⁹ Recently, NICS analyses of the $\text{Au}_{20}(\text{SR})_{16}$ cluster were performed to support the concept of a superatom-network (SAN);⁵⁰ a theory to explain the stability of thiolate-protected gold nanoclusters. Thus, it is sensible to examine the stabilities of $\text{Au}_{20}(\text{SR})_{16}$, $\text{Au}_{28}(\text{SR})_{20}$, $\text{Au}_{36}(\text{SR})_{24}$, $\text{Au}_{44}(\text{SR})_{28}$, and $\text{Au}_{52}(\text{SR})_{32}$ based on the computed NICS values corresponding to the center of the tetrahedral Au_4 units of these clusters. It can be seen that the absolute NICS values (see Table 2) at the centers of the tetra-

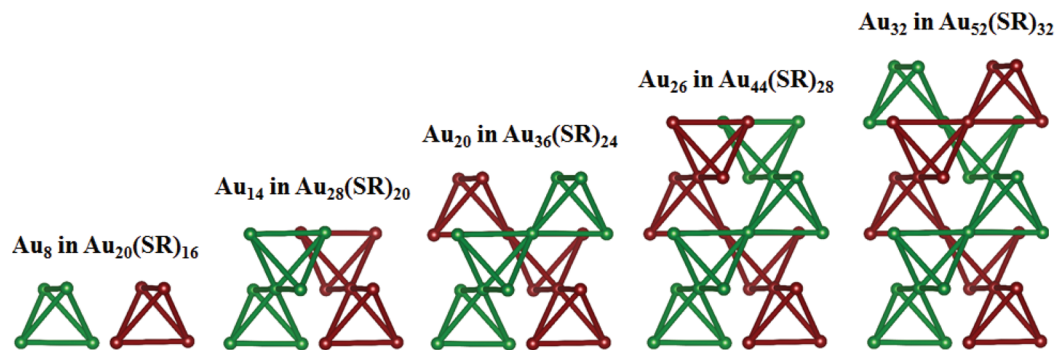


Fig. 2 The structures of Au_8 in $\text{Au}_{20}(\text{SR})_{16}$, Au_{14} in $\text{Au}_{28}(\text{SR})_{20}$, Au_{20} in $\text{Au}_{36}(\text{SR})_{24}$, Au_{26} in $\text{Au}_{44}(\text{SR})_{28}$, and Au_{32} in $\text{Au}_{52}(\text{SR})_{32}$. Au atoms are both olive and wine.

Table 2 Computed nucleus-independent chemical shift (NICS) values of $\text{Au}_{20}(\text{SR})_{16}$, $\text{Au}_{28}(\text{SR})_{20}$, $\text{Au}_{36}(\text{SR})_{24}$, $\text{Au}_{44}(\text{SR})_{28}$, and $\text{Au}_{52}(\text{SR})_{32}$. "0" denotes the NICS values at the centers of the total structures. "1–10" denote the NICS values at the centers of tetrahedral Au_4 units of these clusters (ESI Fig. S3)

| | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|----------------------------------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| $\text{Au}_{20}(\text{SR})_{16}$ | −7.5 | −28.2 | −28.7 | | | | | | | | |
| $\text{Au}_{28}(\text{SR})_{20}$ | −12.4 | −25.3 | −26.3 | −25.2 | −26.5 | | | | | | |
| $\text{Au}_{36}(\text{SR})_{24}$ | −10.8 | −24.5 | −26.2 | −23.4 | −25.1 | −24.2 | −25.7 | | | | |
| $\text{Au}_{44}(\text{SR})_{28}$ | −17.3 | −25.6 | −23.5 | −23.5 | −25.6 | −25.6 | −23.8 | −23.5 | −25.6 | | |
| $\text{Au}_{52}(\text{SR})_{32}$ | −12.7 | −25.9 | −25.1 | −24.2 | −22.1 | −25.5 | −26.0 | −23.1 | −23.0 | −24.7 | −25.7 |

hedral Au_4 units are large; larger than those at the centers of the total structures. The NICS results suggest notable aromaticity in the tetrahedral Au_4 units. As such, the overall stabilities of $\text{Au}_{20}(\text{SR})_{16}$, $\text{Au}_{28}(\text{SR})_{20}$, $\text{Au}_{36}(\text{SR})_{24}$, $\text{Au}_{44}(\text{SR})_{28}$, and $\text{Au}_{52}(\text{SR})_{32}$ likely stem from the local stability of each tetrahedral Au_4 unit.

The unique growth-pattern rule derived among the series of clusters, $\text{Au}_{20}(\text{SR})_{16}$, $\text{Au}_{28}(\text{SR})_{20}$, $\text{Au}_{36}(\text{SR})_{24}$, $\text{Au}_{44}(\text{SR})_{28}$ and $\text{Au}_{52}(\text{SR})_{32}$, suggests the possible existence of larger-sized clusters through continuously adding the motif $[\text{Au}_8(\text{SR})_4]$, e.g., $\text{Au}_{52}(\text{SR})_{32} + [\text{Au}_8(\text{SR})_4] \rightarrow \text{Au}_{60}(\text{SR})_{36} + [\text{Au}_8(\text{SR})_4] \rightarrow \text{Au}_{68}(\text{SR})_{40} + [\text{Au}_8(\text{SR})_4] \rightarrow \text{Au}_{76}(\text{SR})_{44}$, where the newly created $\text{Au}_{60}(\text{SR})_{36}$, $\text{Au}_{68}(\text{SR})_{40}$, and $\text{Au}_{76}(\text{SR})_{44}$ all possess the FCC-type Au-kernels (Fig. 3). Fig. 4 presents the computed HOMO–LUMO gaps of the optimized nanoclusters from the small-sized $\text{Au}_{20}(\text{SR})_{16}$ to large-sized $\text{Au}_{76}(\text{SR})_{44}$, as well as the experimentally measured optical gaps of $\text{Au}_{20}(\text{SR})_{16}$, $\text{Au}_{28}(\text{SR})_{20}$, $\text{Au}_{36}(\text{SR})_{24}$, and $\text{Au}_{44}(\text{SR})_{28}$. The computed gaps reproduce the experimental gaps quite well except for $\text{Au}_{28}(\text{SR})_{20}$. Nevertheless, the computed gap of $\text{Au}_{28}(\text{SR})_{20}$ is consistent with a previous theoretical study.¹⁴ The HOMO–LUMO gaps of $\text{Au}_{60}(\text{SR})_{36}$, $\text{Au}_{68}(\text{SR})_{40}$, and $\text{Au}_{76}(\text{SR})_{44}$ are all greater than 1.0 eV, comparable to those of $\text{Au}_{64}(\text{SC}_6\text{H}_{11})_{32}$ ⁵¹ and $\text{Au}_{67}(\text{PET})_{35}$.⁵² Double-helix structures made of tetrahedral Au_4 units can be seen in the three new structures (ESI Fig. S4†), and are also present in $\text{Au}_{20}(\text{SR})_{16}$, $\text{Au}_{28}(\text{SR})_{20}$, $\text{Au}_{36}(\text{SR})_{24}$, $\text{Au}_{44}(\text{SR})_{28}$ and $\text{Au}_{52}(\text{SR})_{32}$ clusters. Furthermore, the NICS analyses (ESI Table S1 and Fig. S6†) also show that the overall stabilities of $\text{Au}_{60}(\text{SR})_{36}$, $\text{Au}_{68}(\text{SR})_{40}$, and $\text{Au}_{76}(\text{SR})_{44}$ are likely due to the local stability

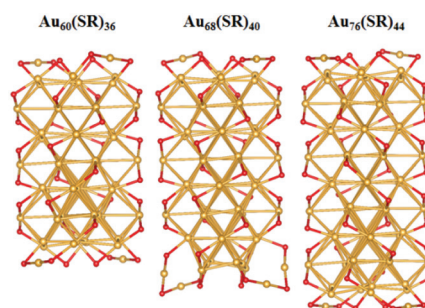


Fig. 3 The optimized structures of $\text{Au}_{60}(\text{SR})_{36}$, $\text{Au}_{68}(\text{SR})_{40}$, and $\text{Au}_{76}(\text{SR})_{44}$, where the methyl groups are omitted for clarity. Au and S atoms are in gold and red, respectively.

of each tetrahedral Au_4 unit. The large HOMO–LUMO gaps and the negative NICS values suggest high stability of the newly predicted structures.

It should be noted that the $\text{Au}_{76}(4\text{-MEBA})_{44}$ (4-MEBA = 4-(2-mercaptoethyl)benzoic acid) nanocluster has been synthesized recently by Takano *et al.*⁵³ Although $\text{Au}_{76}(4\text{-MEBA})_{44}$ has the same number of Au atoms and ligands as $\text{Au}_{76}(\text{SR})_{44}$, a comparison of the computed and experimental X-ray diffraction (XRD) and optical absorption spectra suggests that the two clusters may have different structures in their Au-kernels (ESI Fig. S5†). It is known that surface-protecting thiolates can have significant effects on the structures of gold nanoclusters even with the same number of Au and S atoms. For example, the marked differences in their absorption spectra indicate that



Fig. 4 The computed HOMO–LUMO gaps of the optimized nanoclusters from small-sized Au₂₀(SR)₁₆ to large-sized Au₇₆(SR)₄₄, and the measured optical gaps.

Au₄₀(*o*-MBT)₂₄⁴³ and Au₄₀(PET)₂₄⁴⁴ have different structures, and so do Au₂₀(PET)₁₆³² and Au₂₀(TBBT)₁₆,⁸ as well as Au₂₈(TBBT)₂₀¹³ and Au₂₈(S-*c*-C₆H₁₁)₂₀.⁴⁰ Moreover, even with the same ligands, different Au₃₈(PET)₂₄ isomers have been detected.^{15,54}

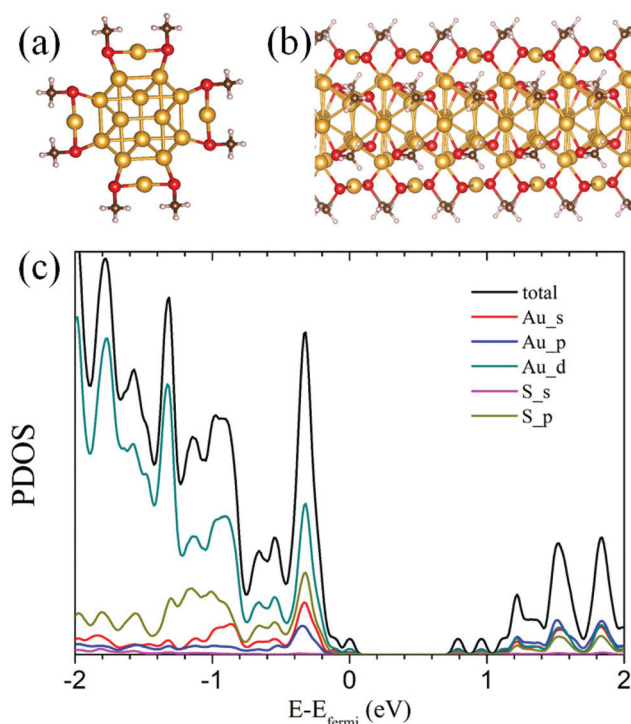


Fig. 5 The proposed structure of the thiolate-protected gold nanowire: (a) viewed along the wire; (b) side view. Au, S, C, and H atoms are in gold, red, dark gray, and white, respectively. (c) Computed projected density of state (PDOS) of the thiolate-protected gold nanowire. Au_s, Au_p, and Au_d denote the s, p, and d orbitals of Au atoms, respectively. S_s and S_p denote the s and p orbitals of S atoms, respectively.

Lastly, if the growth-pattern rule is extended to the infinitely-long nanowire limit by repeatedly adding [Au₈(SR)₄] units in one direction, the thiolate-protected gold nanowire (RS-AuNW) can be obtained, as shown in Fig. 5(a) and (b). The present RS-AuNW also exhibits a double-helix structure made of tetrahedral Au₄ units, which is very different from that of previously proposed vertex- and face-sharing icosahedral thiolated Au nanowires⁵⁵ and crystallized [Au₂₅(SBu)₁₈]_n nanowires.⁵⁶ Fig. 5(c) shows the computed total density of state (DOS) of the present RS-AuNW, which shows an electronic band gap of 0.78 eV, suggesting that the present RS-AuNW is semiconducting. The vertex-sharing thiolated gold nanowire can be made either semiconducting or metallic by tuning the charge. The face-sharing nanowire is always metallic. The non-magnetic ground state of [Au₂₅(SBu)₁₈]_n has a band gap of 0.12 eV, suggesting that [Au₂₅(SBu)₁₈]_n could behave as a narrow-gap semiconductor. It is also found that the valence band of the present RS-AuNW is mainly contributed to by the Au(5d), S(3p) Au(6s), and Au(6p) atomic orbitals, while the conduction band is mainly due to the Au(6sp) atomic orbitals.

Conclusions

In conclusion, a generic growth-pattern rule is identified based on the series of nanoclusters Au₂₀(SR)₁₆, Au₂₈(SR)₂₀, Au₃₆(SR)₂₄, Au₄₄(SR)₂₈, and Au₅₂(SR)₃₂, which can be viewed as the sequential addition of [Au₈(SR)₄] units. The large negative nucleus-independent chemical shift (NICS) values in the centers of the tetrahedral Au₄ units indicate that the integral stabilities of these clusters are determined by the local stability of each tetrahedral Au₄ unit. Extension of the rule to larger-sized nanoclusters than the state-of-the-art gives rise to new structures of nanoclusters such as Au₆₀(SR)₃₆, Au₆₈(SR)₄₀, and Au₇₆(SR)₄₄. All three large-sized nanoclusters exhibit relatively large HOMO–LUMO gaps and negative NICS values, suggesting their high chemical stability. It is also found that the computed XRD and optical absorption spectra of Au₇₆(SR)₄₄ are not the same as those of Au₇₆(4-MEBA)₄₄ from experiments, suggesting the two nanoclusters may have different Au-kernel structures. Finally, extension of the growth-pattern rule to the infinitely long nanowire limit results in a 1D RS-AuNW with a band gap of 0.78 eV. The unique growth-pattern rule offers a guide for future synthesis of a new class of large-sized thiolate-protected gold nanoclusters or even RS-AuNW that has not been reported in the literature.

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Electronic Supplementary Materials

Unraveling a Generic Growth Pattern in Structure Evolution of Thiolate-Protected Gold Nanoclusters

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Fig. S1. Optimized structures of Au₂₀(SR)₁₆, Au₂₈(SR)₂₀, Au₃₆(SR)₂₄, Au₄₄(SR)₂₈, Au₅₂(SR)₃₂, Au₆₀(SR)₃₆, Au₆₈(SR)₄₀, and Au₇₆(SR)₄₄. Red and yellow denote S and Au atoms, respectively. Methyl groups are omitted for clarity.

Fig. S2. The structures of Au₂₈(S-c-C₆H₁₁)₂₀ (a), Au₂₈(TBBT)₂₀ (c), and their Au₂₀ kernels (b and d). Red and yellow denote S and Au atoms in the staple, respectively. The Au₂₀ kernels are in olive. Ligands are omitted for clarity.

Fig. S3. Computed nucleus-independent chemical shift (NICS) grid for Au₂₀(SR)₁₆, Au₂₈(SR)₂₀, Au₃₆(SR)₂₄, Au₄₄(SR)₂₈, and Au₅₂(SR)₃₂ clusters. Olive and yellow denote S and Au atoms, respectively. The tetrahedron Au₄ units are in red. The green (0) and blue (1-10) balls denote the centers of total structure and the tetrahedron Au₄ unit, respectively.

Fig. S4. The double-helix structures of Au₃₈ in Au₆₀(SR)₃₆, Au₄₄ in Au₆₈(SR)₄₀, and Au₅₀ in Au₇₆(SR)₄₄. The Au atoms are in olive and wine, respectively.

Fig. S5. Computed (red line) and experimental (black line) (a) XRD and (b) optical absorption spectra.

Fig. S6. Computed nucleus-independent chemical shift (NICS) grid for Au₆₀(SR)₃₆, Au₆₈(SR)₄₀, and Au₇₆(SR)₄₄ clusters. Olive and yellow denote S and Au atoms, respectively. The tetrahedron Au₄ units are in red. The green (0) and blue (1-16) balls denote the centers of total structure and the tetrahedron Au₄ unit, respectively.

Table S1. Computed nucleus-independent chemical shift (NICS) values of Au₆₀(SR)₃₆, Au₆₈(SR)₄₀, and Au₇₆(SR)₄₄. “0” denotes the NICS values at the center of the total structures. “1-16” denote the NICS values at the centers of tetrahedron Au₄ units of these clusters (ESI Fig. S6).

Coordinates file of optimized structure of Au₆₀(SCH₃)₃₆

Coordinates file of optimized structure of Au₆₈(SCH₃)₄₀

Coordinates file of optimized structure of Au₇₆(SCH₃)₄₄

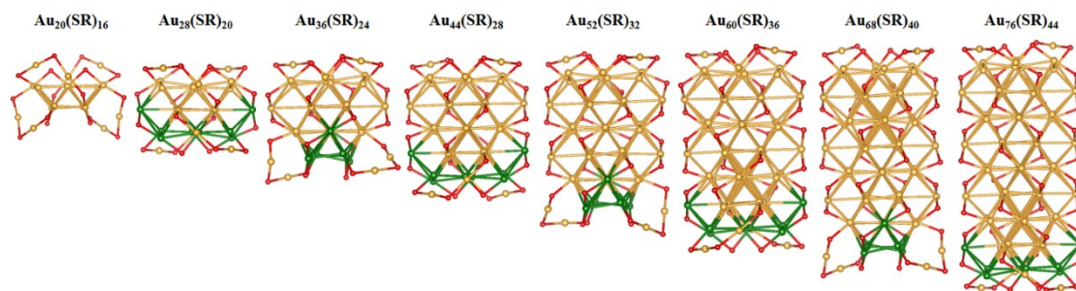


Fig. S1. Optimized structures of $\text{Au}_{20}(\text{SR})_{16}$, $\text{Au}_{28}(\text{SR})_{20}$, $\text{Au}_{36}(\text{SR})_{24}$, $\text{Au}_{44}(\text{SR})_{28}$, $\text{Au}_{52}(\text{SR})_{32}$, $\text{Au}_{60}(\text{SR})_{36}$, $\text{Au}_{68}(\text{SR})_{40}$, and $\text{Au}_{76}(\text{SR})_{44}$. Red and yellow denote S and Au atoms, respectively. Methyl groups are omitted for clarity.

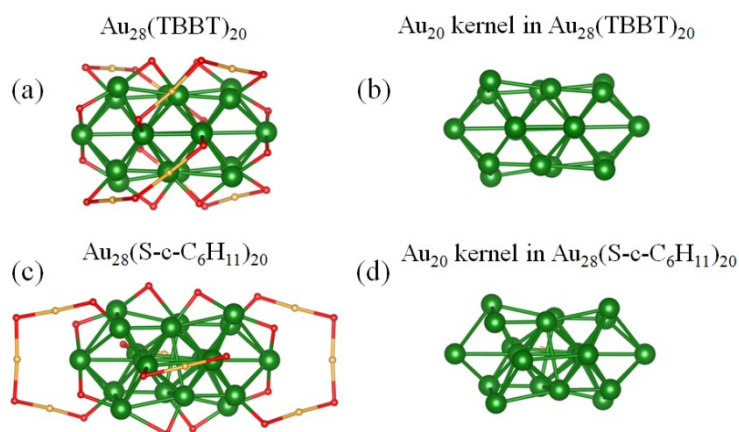


Fig. S2. The structures of $\text{Au}_{28}(\text{S-c-C}_6\text{H}_{11})_{20}$ (a), $\text{Au}_{28}(\text{TBBT})_{20}$ (c), and their Au_{20} kernels (b and d). Red and yellow denote S and Au atoms in the staple, respectively. The Au_{20} kernels are in olive. Ligands are omitted for clarity.

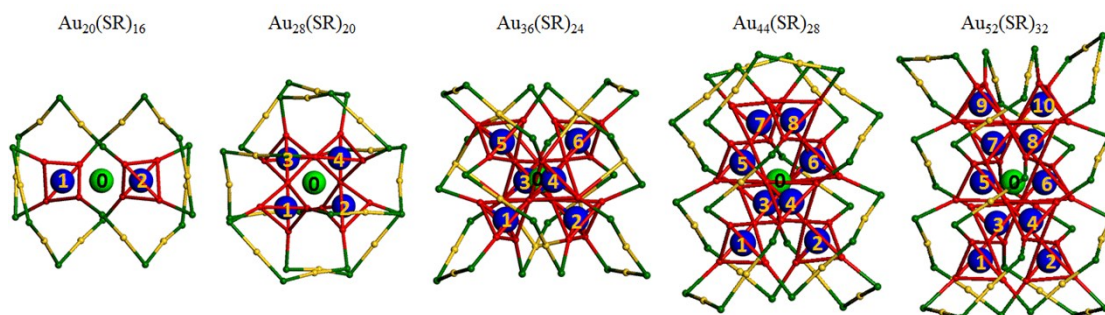


Fig. S3. Computed nucleus-independent chemical shift (NICS) grid for $\text{Au}_{20}(\text{SR})_{16}$, $\text{Au}_{28}(\text{SR})_{20}$, $\text{Au}_{36}(\text{SR})_{24}$, $\text{Au}_{44}(\text{SR})_{28}$, and $\text{Au}_{52}(\text{SR})_{32}$ clusters. Olive and yellow denote S and Au atoms, respectively. The tetrahedron Au_4 units are in red. The green (0) and blue (1-10) balls denote the centers of total structure and the tetrahedron Au_4 unit, respectively.

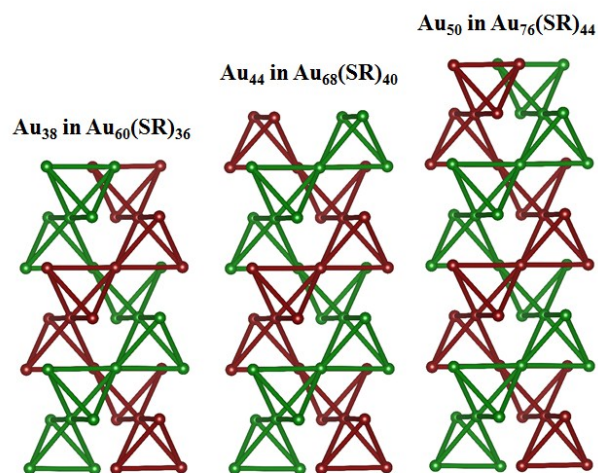


Fig. S4. The double-helix structures of Au_{38} in $\text{Au}_{60}(\text{SR})_{36}$, Au_{44} in $\text{Au}_{68}(\text{SR})_{40}$, and Au_{50} in $\text{Au}_{76}(\text{SR})_{44}$. The Au atoms are in olive and wine, respectively.

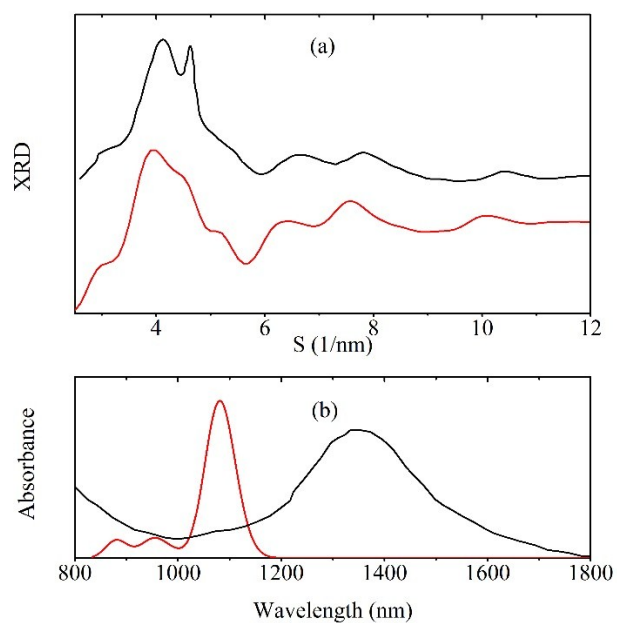


Fig. S5. Computed (red line) and experimental (black line) (a) XRD and (b) optical absorption spectra.

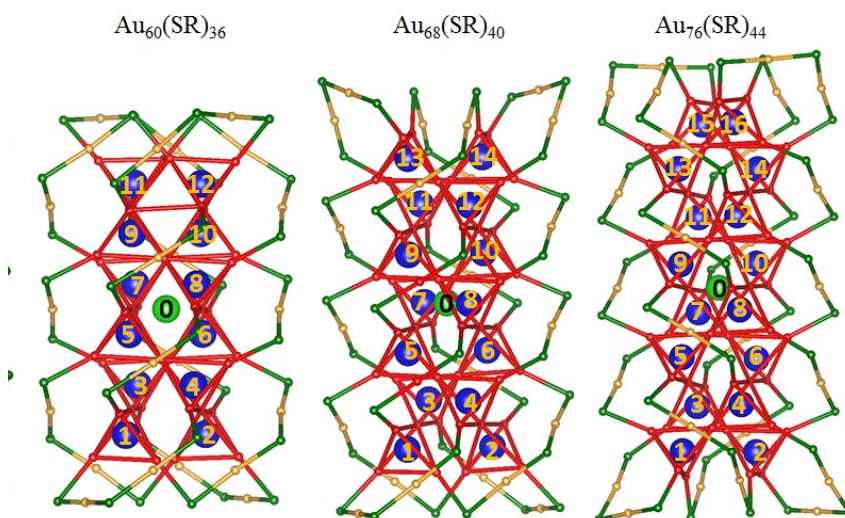


Fig. S6. Computed nucleus-independent chemical shift (NICS) grid for $\text{Au}_{60}(\text{SR})_{36}$, $\text{Au}_{68}(\text{SR})_{40}$, and $\text{Au}_{76}(\text{SR})_{44}$ clusters. Olive and yellow denote S and Au atoms, respectively. The tetrahedron Au_4 units are in red. The green (0) and blue (1-16) balls denote the centers of total structure and the tetrahedron Au_4 unit, respectively.

Table S1. Computed nucleus-independent chemical shift (NICS) values of $\text{Au}_{60}(\text{SR})_{36}$, $\text{Au}_{68}(\text{SR})_{40}$, and $\text{Au}_{76}(\text{SR})_{44}$. “0” denotes the NICS values at the center of the total structures. “1-16” denote the NICS values at the centers of tetrahedron Au_4 units of these clusters (ESI Fig. S6).

| | $\text{Au}_{60}(\text{SR})_{36}$ | $\text{Au}_{68}(\text{SR})_{40}$ | $\text{Au}_{76}(\text{SR})_{44}$ |
|----|----------------------------------|----------------------------------|----------------------------------|
| 0 | -15.6 | -9.7 | -15.1 |
| 1 | -25.5 | -23.4 | -24.5 |
| 2 | -24.0 | -22.0 | -21.1 |
| 3 | -23.9 | -22.1 | -20.8 |
| 4 | -22.0 | -24.0 | -24.0 |
| 5 | -21.3 | -24.1 | -22.7 |
| 6 | -25.2 | -24.2 | -19.2 |
| 7 | -26.5 | -26.7 | -21.4 |
| 8 | -22.6 | -25.1 | -27.9 |
| 9 | -23.7 | -23.1 | -26.9 |
| 10 | -24.0 | -20.8 | -23.1 |
| 11 | -22.4 | -23.5 | -21.8 |
| 12 | -25.8 | -23.1 | -21.1 |
| 13 | | -24.5 | -18.8 |
| 14 | | -25.8 | -22.0 |
| 15 | | | -24.0 |
| 16 | | | -26.6 |

Coordinates of the optimized structure of Au₆₀(SCH₃)₃₆

| | | | |
|----|--------------|--------------|--------------|
| Au | 17.122707048 | 4.404385117 | 25.201650990 |
| Au | 14.486219184 | 3.471272597 | 26.314130598 |
| Au | 16.326299973 | 1.452006454 | 24.891069256 |
| Au | 14.833251322 | 3.443896836 | 23.292916987 |
| Au | 16.931743602 | 4.338248168 | 28.105233061 |
| Au | 15.887734923 | 1.555299472 | 27.833564944 |
| Au | 12.315527616 | 2.453256387 | 24.249125914 |
| Au | 16.731513588 | 1.411276358 | 21.905771177 |
| Au | 15.052150645 | 6.297644304 | 26.620923421 |
| Au | 17.235840616 | 1.587450055 | 19.118350560 |
| Au | 13.070383233 | 2.812941121 | 18.082714115 |
| Au | 19.736041069 | 2.386332135 | 20.714158594 |
| Au | 14.089709735 | 0.547265915 | 23.002085600 |
| Au | 17.220117822 | -3.832557345 | 23.451820410 |
| Au | 12.756621450 | 2.607989455 | 21.485827123 |
| Au | 11.468271780 | 7.947492382 | 27.788657227 |
| Au | 12.939436545 | 5.562273061 | 24.984701542 |
| Au | 20.121637195 | 5.441429358 | 24.042320289 |
| Au | 13.880421864 | 0.670626879 | 26.100089090 |
| Au | 18.613015792 | 2.517181901 | 26.863394470 |
| Au | 13.261704620 | 8.923055167 | 24.732875197 |
| Au | 13.118156416 | 5.649261554 | 21.539005008 |
| Au | 15.604210876 | 6.208594809 | 23.658162368 |
| Au | 14.108967085 | 3.397278071 | 29.753431261 |
| Au | 18.858390635 | 2.209097923 | 23.648012010 |
| Au | 17.324714079 | 4.435326756 | 22.342855120 |
| Au | 17.959353140 | 7.707644225 | 25.552974208 |
| Au | 12.776883876 | 5.161004860 | 27.784283216 |
| Au | 11.194250970 | -0.375320525 | 24.292578277 |
| Au | 15.421335464 | -1.538283650 | 24.496215616 |
| Au | 14.537766056 | 0.581686327 | 19.935342963 |
| Au | 19.238206692 | 5.281909957 | 26.843263888 |
| Au | 15.416017792 | 3.362648951 | 20.277415762 |
| Au | 18.071636173 | -0.478864813 | 23.634711751 |
| Au | 15.799877493 | -1.529392805 | 21.633258526 |
| Au | 11.474100796 | 2.496901000 | 27.575836144 |
| Au | 13.237936017 | -2.163942699 | 22.864454894 |
| Au | 17.976436244 | -0.732851244 | 26.678207677 |
| Au | 18.678102935 | 1.804787870 | 30.293106977 |
| Au | 20.803633075 | 4.700684158 | 29.452277517 |
| S | 20.970115188 | 3.274362939 | 24.359074176 |

| | | | |
|----|--------------|--------------|--------------|
| S | 20.543048850 | 0.183019244 | 20.392186036 |
| S | 19.293724451 | 4.703766977 | 20.913993965 |
| S | 15.224116824 | -5.100633700 | 23.544094465 |
| S | 11.508412710 | 9.614215299 | 26.151921485 |
| S | 10.416954161 | 3.233867306 | 25.613739080 |
| S | 10.123445154 | 0.295148984 | 22.285977006 |
| S | 16.013040279 | -2.029888901 | 26.840624462 |
| S | 19.978684877 | 0.518056785 | 26.587034621 |
| S | 16.860709207 | 0.420687048 | 29.776041790 |
| S | 14.869431102 | 2.855566693 | 16.546870455 |
| S | 11.382673865 | 5.714870470 | 23.139258116 |
| S | 12.378755992 | 1.782774351 | 29.648261940 |
| S | 11.918954586 | -0.743186015 | 26.516671446 |
| S | 11.236583268 | 2.785899706 | 19.571122027 |
| S | 14.508910589 | 5.560422644 | 19.637578141 |
| S | 14.761164743 | 8.412502586 | 23.004865416 |
| S | 19.255171543 | -2.633206429 | 23.403795248 |
| S | 21.047041460 | 6.507305272 | 27.967051461 |
| S | 20.703202968 | 2.860408393 | 30.889225932 |
| S | 11.251896424 | 6.238228095 | 29.388498210 |
| S | 19.439623542 | 7.683085591 | 23.708380568 |
| Au | 18.320477278 | -0.815690304 | 20.577180890 |
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| Au | 16.367937206 | -1.482188959 | 18.624411700 |
| Au | 13.661005674 | -2.335315525 | 19.668247283 |
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| Au | 16.963577647 | -1.469770843 | 15.868177725 |
| Au | 12.704804686 | -4.945303484 | 19.365149171 |
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| S | 17.816666216 | -1.642502703 | 13.592398691 |
| Au | 12.352851865 | -0.127978247 | 14.307805332 |
| Au | 15.593165718 | -1.155885775 | 12.991331231 |
| S | 13.435297097 | -0.597245320 | 12.271023584 |
| S | 11.474664584 | -7.030952360 | 19.006174677 |
| S | 18.692940803 | -5.574877254 | 20.797716185 |
| Au | 13.556883655 | -7.976993167 | 19.555415680 |
| Au | 17.060899149 | -7.197271580 | 20.362670180 |
| S | 15.539801918 | -8.995441315 | 20.249594014 |
| S | 18.487516674 | 1.630813769 | 16.992887531 |

| | | | |
|----|--------------|---------------|--------------|
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| C | 16.102880295 | 9.650078077 | 23.154507405 |
| C | 20.876894151 | 8.643293779 | 24.334544371 |
| C | 22.303352883 | 3.138666586 | 23.104067604 |
| C | 18.801344304 | 5.280892486 | 19.248877355 |
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| C | 20.112464150 | -3.005365718 | 24.979256957 |
| C | 20.901722322 | 0.119530164 | 28.120314150 |
| C | 16.560259074 | -3.774820810 | 26.944211401 |
| C | 15.721912721 | 0.574162098 | 31.203639768 |
| C | 12.113420603 | 11.128034657 | 26.993389492 |
| C | 12.318661226 | 6.765653851 | 30.786972045 |
| C | 10.635188808 | 7.382874572 | 22.996286264 |
| C | 8.964946799 | 2.133520171 | 25.405368877 |
| C | 11.156405409 | 2.429465515 | 30.858342303 |
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| C | 14.137692794 | 3.060777118 | 14.878502304 |
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| C | 12.722068575 | -2.209785135 | 11.752765197 |
| C | 17.958728526 | -3.443995781 | 13.254137754 |
| C | 19.991577967 | 2.680717023 | 17.077058089 |
| C | 21.300006785 | -2.787801189 | 15.948758822 |
| C | 16.987413655 | -6.866731267 | 16.747547218 |
| C | 13.055277294 | -5.232562443 | 15.452689212 |
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Coordinates file of optimized structure of Au₆₈(SCH₃)₄₀

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| Au | 19.804491238 | 5.617599725 | 24.066164660 |
| Au | 13.835318391 | 0.627408419 | 26.103908749 |
| Au | 18.443284060 | 2.697740184 | 26.989833100 |
| Au | 14.619107798 | 4.707500813 | 33.524674112 |
| Au | 12.965763135 | 5.587081703 | 21.555414559 |
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| S | 16.844860165 | 3.962740238 | 33.437015391 |
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| S | 19.145583265 | 4.820329570 | 20.908662972 |
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Coordinates of the optimized structure of Au₇₆(SCH₃)₄₄

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| Au | 14.406185599 | 3.161392825 | 26.611765110 |
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| Au | 14.429355704 | 3.127339129 | 23.551895135 |
| Au | 17.354323962 | 7.228243372 | 28.446990288 |
| Au | 16.711863804 | 4.252383225 | 28.265162552 |
| Au | 17.206874769 | 7.287837304 | 31.526295277 |
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| Au | 14.931056809 | 6.286308874 | 29.841486577 |
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| Au | 15.570208500 | 9.247019317 | 29.984027988 |
| Au | 15.399990706 | 9.301243007 | 32.953598466 |
| Au | 16.360714689 | 12.203557448 | 33.029922912 |
| Au | 16.374231031 | 1.451647392 | 18.417569803 |
| Au | 17.985352587 | -0.217700192 | 20.402031844 |
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| Au | 11.990023479 | 1.747700933 | 21.915365448 |
| Au | 12.693619979 | 4.873363675 | 25.034254710 |
| Au | 13.116680922 | 8.228759616 | 25.143388214 |
| Au | 19.449562748 | 5.422307669 | 23.582607007 |
| Au | 20.076821460 | 8.290523253 | 26.889329635 |
| Au | 13.806437306 | 11.410359811 | 28.313178513 |
| Au | 20.811782677 | 11.331720500 | 30.197062941 |
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| Au | 18.463837098 | 2.414989268 | 26.513967140 |
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| Au | 18.932503746 | 5.335060488 | 29.853241083 |
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| Au | 14.807855740 | 6.282254439 | 32.704571785 |
| Au | 19.327605377 | 8.161960081 | 33.177367038 |
| Au | 14.957738024 | 9.362997252 | 35.689233494 |
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