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Atomically precise thiolate-protected gold nanomolecules have attracted interest due to their distinct electronic and chemical properties. The structure of these nanomolecules is important for understanding their peculiar properties. Here, we report the X-ray crystal structure of a 24-atom gold nanomolecule protected by 16 *tert*-butylthiolate ligands. The composition of $Au_{24}(S\text{-}C_4H_9)_{16}$ {poly[hexadecakis(μ-*tert*-butylthiolato)tetracosagold]} was confirmed by X-ray crystallography and electrospray ionization mass spectrometry (ESI–MS). The nanomolecule was synthesized in a one-phase synthesis and crystallized from a hexane–ethanol layered solution. The X-ray structure confirms the 16-atom core protected by two monomeric and two trimeric staples with four bridging ligands. The $Au_{24}(S\text{-}C_4H_9)_{16}$ cluster follows the shell-closing magic number of 8.

1. Introduction

Gold nanomolecules (AuNM) in the 1–3 nm size range exhibit size-dependent molecule-like properties (Rambukwella *et al.*, 2018) and have gained broad interest due to their applications in imaging (Boisselier & Astruc, 2009), catalytic activity (Wang *et al.*, 2005; Wu *et al.*, 2018; Du *et al.*, 2019), biosensing (Saha *et al.*, 2012), and drug delivery (Wey & Epple, 2020; Bowman *et al.*, 2008; Brown *et al.*, 2010). This is due to the stability of AuNMs under ambient conditions, monodispersity, and distinctive optical and electronic properties (Murray, 2008; Chaki *et al.*, 2008; Levi-Kalisman *et al.*, 2011; Tlahuice-Flores *et al.*, 2013; Alvarez *et al.*, 1997). The physicochemical understanding of AuNMs is obstructed by the lack of structural information and information about the atom arrangement. To date, several AuNM crystal structures have been reported (Heaven *et al.*, 2008; Crasto, Barcaro *et al.*, 2014; Crasto, Malola *et al.*, 2014; Dass *et al.*, 2015; Sakthivel *et al.*, 2017, 2020; Das *et al.*, 2013). The AuNM structure consists of three main parts: (i) a metallic core, (ii) staple motifs, and (iii) bridging ligands. The metallic core possesses two types of Au atoms: an inner core where no Au atoms are bonded directly to the ligand and the surface core Au atoms which are bonded directly to the protecting ligand. While the core Au atoms possess a zero oxidation state, the surface core Au atoms have a +1 oxidation state. The staple motifs, where the oxidation number of the Au atom is +2, are identified by $Au_n(SR)_{n+1}$. There are three kinds of staples: (i) a monomeric staple having one Au atom bonded to the core *via* two ligands [–S*R*—Au—S*R*–], (ii) dimeric staples where two Au atoms are bonded to the core through three ligands [–S*R*—Au—S*R*—Au—S*R*–], and (iii) trimeric staples which have three Au atoms bonded to the core by four ligands [–S*R*—Au—S*R*—Au—S*R*—Au—S*R*–]. The structure of the core and the arrangement of the ligands

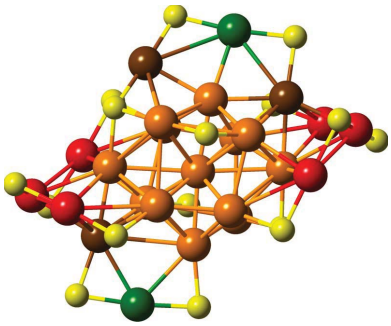

Table 1
Experimental details.

Crystal data	
Chemical formula	$[Au_{24}(C_4H_9S)_{16}]$
M_r	6153.94
Crystal system, space group	Monoclinic, *Cc*
Temperature (K)	120
a, *b*, *c* (Å)	15.5946 (6), 25.9193 (6), 29.7621 (8)
β (°)	100.655 (2)
V (Å^3)	11822.5 (6)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	57.21
Crystal size (mm)	0.08 × 0.04 × 0.02
Data collection	
Diffractometer	Bruker PHOTON-II CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.362, 0.753
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	57304, 21231, 19685
R_{int}	0.074
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.611
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.049, 0.121, 1.01
No. of reflections	21231
No. of parameters	986
No. of restraints	26
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	3.09, −2.63
Absolute structure	Refined as an inversion twin.
Absolute structure parameter	0.42 (2)

Computer programs: *APEX3* (Bruker, 2019), *SAINT* (Bruker, 2019), *SHELXT2018* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*), *OLEX2* (Dolomanov *et al.*, 2009), *CrystalMaker* (Palmer, 2014), and *OLEX2* (Dolomanov *et al.*, 2009).

dictate the stability, electrochemical properties, and composition of the AuNM.

Thiols are the most commonly used ligands in AuNMs. Thiols with differing electronic and steric properties yield a unique series of AuNMs resulting in an AuNM library (Jones *et al.*, 2018; Sakthivel & Dass, 2018; Riccardi *et al.*, 2019; Hesari & Workentin, 2014; Heaven *et al.*, 2008; Yang *et al.*, 2014; Negishi *et al.*, 2005, 2012; Gan *et al.*, 2017; Maman *et al.*, 2020; Das *et al.*, 2013; Crasto, Barcaro *et al.*, 2014; Crasto, Malola *et al.*, 2014; Dass *et al.*, 2015; Sakthivel *et al.*, 2017, 2020). These thiol ligands can be further categorized into three classes: (i) aliphatic thiols such as *n*-butanethiol and aliphatic-like phenylethanethiol, (ii) aromatic thiols such as thiophenol and 4-*tert*-butylbenzenethiol, and (iii) bulky thiols such as *tert*-butylthiol and 1-adamantanethiol. The optical and electrochemical properties, structure, and size of the AuNM are dictated by the type of protecting ligand. In the aromatic thiols, the arene ring and the bulkiness play major roles in determining the properties of the AuNM by forming favorable inter-ligand interactions (Rambukwella *et al.*, 2018). In the case of bulky ligands, the tertiary C atom drives the electron density towards the S atom and thereby forms a stronger Au—S bond (Rambukwella *et al.*, 2018). Larger AuNMs have been synthesized in aliphatic [$Au_{329}(SR)_{84}$ (Kumara & Dass, 2014), $Au_{144}(SR)_{60}$ (Yan *et al.*, 2018), and $Au_{940}(SR)_{160}$ (Kumara *et al.*, 2014)] and aromatic [$Au_{279}(SR)_{84}$ (Sakthivel *et al.*, 2018), $Au_{191}(SR)_{66}$ (Sakthivel *et al.*, 2020), and $Au_{133}(SR)_{52}$ (Dass *et al.*, 2015)] ligand series. The bulky ligand series is limited to a few sizes, such as $Au_{21}(SR)_{15}$ (Xiong *et al.*, 2018), $Au_{23}(SR)_{16}$ (Hesari & Workentin, 2014), $Au_{24}(SR)_{16}$ (Crasto, Barcaro *et al.*, 2014), $Au_{30}(SR)_{18}$ (Crasto & Dass, 2013; Li *et al.*, 2021), $Au_{46}(SR)_{24}$ (Jones *et al.*, 2018), and $Au_{65}(SR)_{29}$ (Jones *et al.*, 2018), due to the steric hindrance induced by the *tert*-butyl group. Here we report the crystal structure of $Au_{24}(S\text{-}C_4H_9)_{16}$ [given as $Au_{24}(S\text{-}t\text{Bu})_{16}$ hereinafter].

2. Experimental

2.1. Materials

$HAuCl_4{\cdot}3H_2O$ (Alfa–Aesar, 99%), *tert*-butylthiol (*t*BuSH) (Acros, 99%), $NaBH_4$ (Acros Organics, 99%), caesium acetate (Acros, 99%), and HPLC-grade solvents [tetrahydrofuran (THF), acetonitrile, methanol, hexane, and dichloromethane] were used as received.

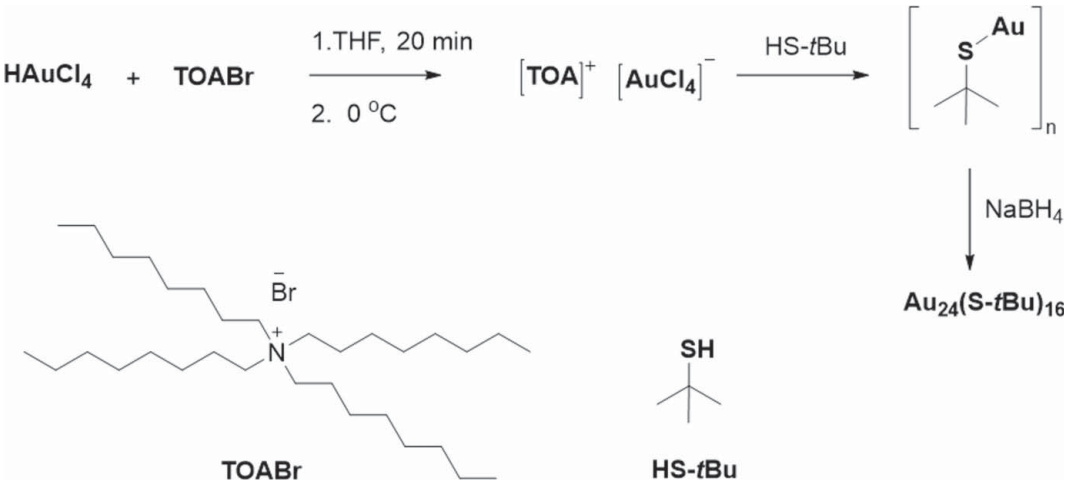

Figure 1
The reaction scheme for the preparation of $Au_{24}(S\text{-}t\text{Bu})_{16}$.

2.2. Synthesis

Briefly (see Fig. 1), the crystal of $Au_{24}(S\text{-}tBu)_{16}$ was obtained from crystallization of an Au:*t*BuSH (1:6) crude dichloromethane-extracted portion (Hesari & Workentin, 2014). In a typical reaction, 0.254 mmol (100 mg, 0.0254 mol l^{-1}) of $HAuCl_4{\cdot}3H_2O$ was mixed with 0.380 mmol (208.2 mg, 0.038 mol l^{-1}) of tetra-*n*-octylammonium bromide in 10 ml of THF in a 100 ml round-bottomed flask (RBF). After 20 min of stirring (500 rpm), the solution was cooled in an ice bath for 30 min. To this cooled solution, 172 µl of *t*BuSH (1:6 $HAuCl_4$:*t*BuSH) was added under slow stirring. The orange color of the solution turned colorless upon addition of the thiol. After 1 h, 25 mmol (96 mg, 25 mol l^{-1}) of $NaBH_4$ dissolved in 1 ml of ice-cold water was added and stirring was continued for 18–26 h. The RBF with the crude solution was then rotary evaporated to dryness. Next, the dried crude was transferred to a 50 ml centrifuge tube and the crude was washed with methanol and water (4–5 times) to remove excess thiol, $NaBH_4$, and other impurities; AuNMs are not soluble in either water or methanol. The AuNM product was then extracted separately, initially with acetonitrile, followed by dichloromethane. The negatively charged small AuNM species are dissolved in acetonitrile while other AuNM species are dissolved in dichloromethane. The samples in acetonitrile and dichloromethane were rotary evaporated to dryness and stored in a refrigerator.

2.3. Mass spectrometry

Electrospray ionization mass spectrometry (ESI–MS) was carried out for the identification of the nanomolecules. The ESI–MS spectra were obtained on a Waters Synapt XS instrument. The sample was dissolved in THF (2 mg l^{-1}), and the data were collected in both positive and negative modes. A 50 m*M* caesium acetate (CsOAc) solution was added to the sample (sample: CsOAc 1:50 *v*/*v*) to ionize the neutral species present.

2.4. X-ray crystallography

Crystal data, data collection, and structure refinement details are summarized in Table 1. The crystals of $Au_{24}(S\text{-}tBu)_{16}$ were obtained from the dichloromethane-extracted product. The dichloromethane-extracted product was dried and redissolved in 2 ml hexane in a 20 ml glass vial, layered with ethanol (1 ml), capped tight, and kept in a dark undisturbed location at room temperature. After 7–10 d, dark metallic brown plate-like crystals were observed (Fig. S1 in the supporting information). Suitable crystals were selected under an optical microscope and mounted on a Bruker PHOTON-II CMOS diffractometer.

H atoms were added at calculated positions by *OLEX2* (Dolomanov *et al.*, 2009). The crystal was found to be an inversion twin and was refined with a twin domain ratio of 0.58:0.42. A solvent mask was applied to the model accounting for 360 electrons in a void volume of 1556 Å^3 (see Table S8 in the supporting information for details).

3. Results and discussion

Single-crystal X-ray diffraction (sc-XRD) analysis reveals that $Au_{24}(S\text{-}tBu)_{16}$ crystallizes in the monoclinic space group *Cc*. Details of the final refinement can be found in Table 1. The structure of the cluster is shown in Figs. 2 and 3. The arrangement of the core cluster is depicted in Fig. 3(*a*). In the figures, some Au—Au bonds in the staples have been omitted for clarity.

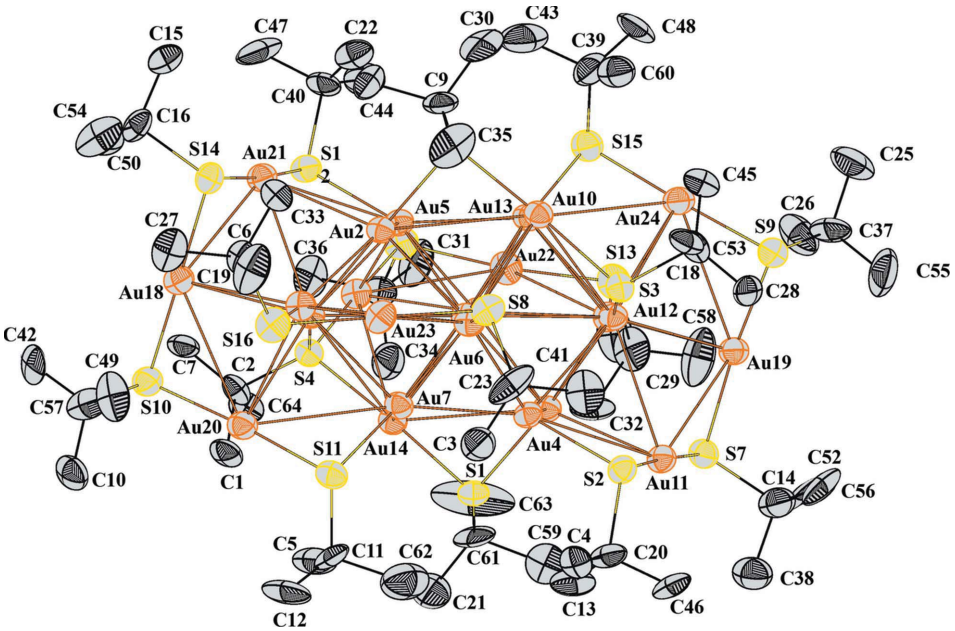

Figure 2
The single-crystal X-ray structure of $Au_{24}(S\text{-}tBu)_{16}$. The Au atoms are shown in orange, S atoms are in yellow, and C atoms are in black. H atoms have been omitted for clarity. Displacement ellipsoids are drawn at the 50% probability level.

The $Au_{24}(S\text{-}tBu)_{16}$ structure is composed of one central Au atom which is bonded to 12 surrounding Au atoms to form a distorted Au_{13} cuboctahedral core [Fig. 3(*a*)]. Three Au atoms cap three 100 faces of the Au_{13} cuboctahedron and give rise to the Au_{16} core [Fig. 3(*a*)]. The protecting staple ligands of the Au_{16} metal core can be categorized as two monomeric [S*R*—Au—S*R*] and two trimeric [S*R*—Au—S*R*—Au—S*R*—Au—S*R*] staples. The monomeric staples are at the front and back along the plane of the paper [Figs. 2 and 3(*b*)]. The trimeric staples are on the right and left sides of the Au_{16} core in the drawing, as shown in Figs. 2 and 3(*c*). The remainder of the four S*R* ligands protect the Au_{16} core as a μ_2-bridging thiol. The packing modes along the *a*, *b*, and *c* axes are shown in Figs. S2(*a*)–(*c*) (see supporting information). The number of free electrons in a gold nanomolecule can predict the stability of a metal cluster (Walter *et al.*, 2008; Häkkinen & Manninen, 1996). The title nanomolecule is a superatom-like nanomolecule with eight free electrons. It satisfies the shell-closing magic number (Walter *et al.*, 2008). In the *tert*-butylthiol-protected AuNM series, only $Au_{23}(S\text{-}tBu)_{16}^-$ and $Au_{24}(S\text{-}tBu)_{16}$ satisfy the shell-closing magic number of electrons.

The Au—Au and Au—S bond distances have been calculated and tabulated in Table 2. In $Au_{24}(S\text{-}tBu)_{16}$, the Au—Au bond within the cuboctahedron is the shortest, *i.e.* Au(cuboctahedra)—Au(cuboctahedra) is 2.91 ± 0.22 Å, and the bond distance varies in the range 3.36–2.64 Å. The average Au(center)—Au(cuboctahedra) bond distance is 2.95 ± 0.23 Å (largest 3.28, shortest 2.73 Å). The Au(center)—Au(cuboctahedra) bond distance is longer than the bond distance between Au atoms residing in the cuboctahedral surface. Because of this vast variety of bond distances, the Au cuboctahedral core is distorted and unsymmetrical. When moving from the core Au atoms to the staple Au atoms, the bond distance increases: Au(trimeric)—Au(core) is 3.14 ± 0.15 Å and Au(monomeric)—Au(core) is 3.03 ± 0.20 Å. The bond distances between monomeric Au atoms and the core Au atoms are shorter than those between trimeric Au atoms and core Au atoms. The Au(trimeric)—Au(trimeric) bond is the longest at 3.27 ± 0.09 Å. The average Au—Au bond distance in the core is less than the Au—Au bond distance in the trimeric staples. The bond distances between the staple Au and S atoms are similar: Au(trimeric)—S is 2.31 ± 0.01 Å and Au(monomeric)—S is 2.29 ± 0.01 Å. The core Au and bridging S atoms have a greater bond length: Au(core)—S(bridging) is 2.35 ± 0.03 Å.

Table 2
Bond distances (Å) of $Au_{24}(S\text{-}tBu)_{16}$ and $Au_{24}(S\text{-}Adm)_{16}$.

	$Au_{24}(S\text{-}tBu)_{16}$			$Au_{24}(S\text{-}Adm)_{16}$		
	Average	Max	Min	Average	Max	Min
Au(center)—Au(cuboctahedra)	2.95 ± 0.23	3.28	2.70	2.93 ± 0.22	3.27	2.70
Au(cuboctahedra)—Au(cuboctahedra)	2.91 ± 0.22	3.36	2.64	2.92 ± 0.20	3.30	2.66
Au(core)—Au(monomeric)	3.03 ± 0.20	3.29	2.82	3.04 ± 0.12	3.12	2.95
Au(core)—Au(trimeric)	3.14 ± 0.15	3.37	2.92	3.12 ± 0.18	3.38	2.94
Au(trimeric)—Au(trimeric)	3.27 ± 0.09	3.37	3.19	3.25 ± 0.00	3.25	3.25
Au(trimeric)—S	2.31 ± 0.01	2.33	2.29	2.30 ± 0.02	2.34	2.28
Au(monomeric)—S	2.29 ± 0.01	2.30	2.29	2.31 ± 0.01	2.31	2.30
Au(core)—S(bridging)	2.35 ± 0.03	2.41	2.30	2.36 ± 0.05	2.54	2.30
S—C	1.86 ± 0.03	1.92	1.80	1.84 ± 0.00	1.84	1.83

The $Au_{24}(S\text{-}tBu)_{16}$ crystal structure is similar to its 1-adamantanethiol counterpart, $Au_{24}(S\text{-}Adm)_{16}$ (Crasto, Barcaro *et al.*, 2014). Both of these AuNMs have bulky ligand groups, *i.e.* *tert*-butylthiol and 1-adamantanethiol. Therefore, the bond distances between these two nanomolecules are directly compared in Table 2. $Au_{24}(S\text{-}Adm)_{16}$ has an average Au(center)—Au(cuboctahedra) distance of 2.93 ± 0.22 Å (maximum 3.27, minimum 2.70 Å). The Au(core)—Au(core) bond distance is 2.92 ± 0.20 Å, Au(trimeric)—Au(core) is 3.12 ± 0.18 Å, Au(monomeric)—Au(core) is 3.04 ± 0.12 Å, Au(trimeric)—S is 2.30 ± 0.02 Å, Au(monomeric)—S is 2.31 ± 0.01 Å, and Au(core)—S(bridging) is 2.36 ± 0.05 Å. Both $Au_{24}(S\text{-}tBu)_{16}$ and $Au_{24}(S\text{-}Adm)_{16}$ show similar Au(core)—

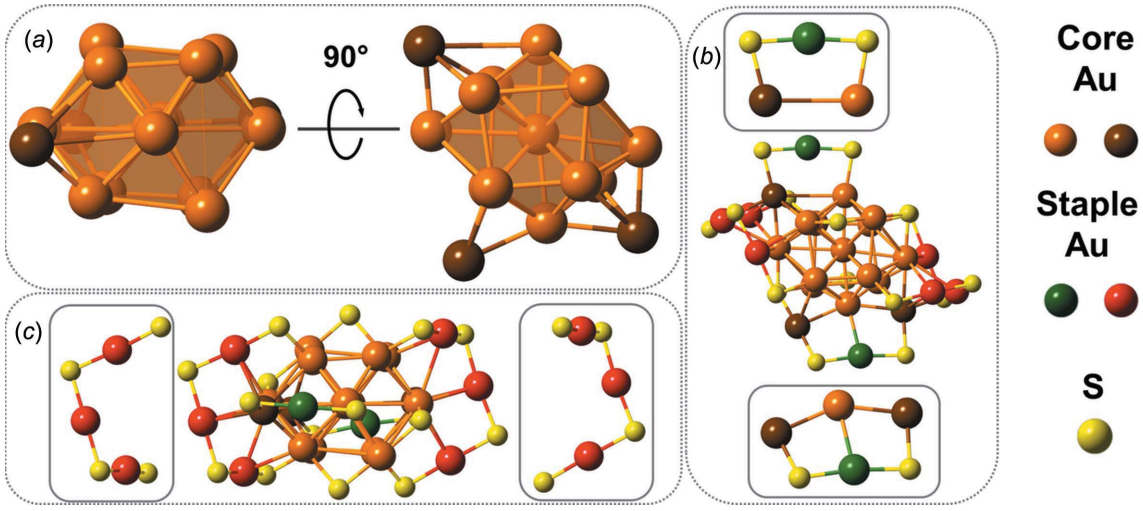

Figure 3
The dissected structure of $Au_{24}(S\text{-}tBu)_{16}$, showing (*a*) the Au_{13} cuboctahedral core capped by three Au atoms, (*b*) the $Au_{24}S_{16}$ structure showing the monomeric staples [S*R*—Au—S*R*], and (*c*) the $Au_{24}S_{16}$ structure showing the trimeric [S*R*—Au—S*R*—Au—S*R*—Au—S*R*] staples. The core Au atoms are shown in orange and brown, the staple Au atoms are shown in green and red, and the S atoms are shown in yellow. C and H atoms have been omitted for clarity.

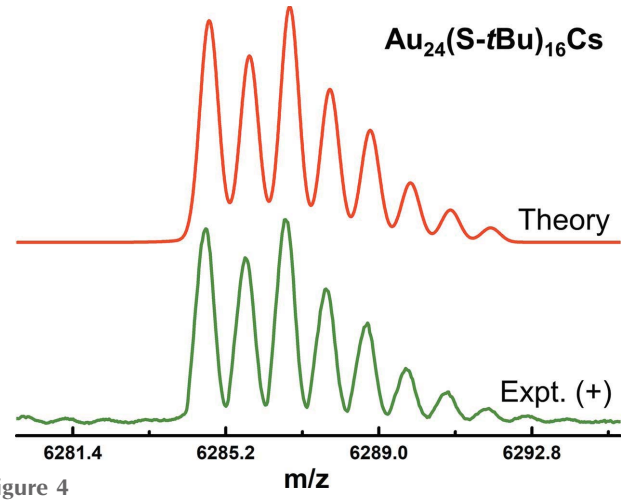

Figure 4
Positive mode ESI–MS spectra [theoretical (red) and experimental (green)] for $Au_{24}(S\text{-}tBu)_{16}$ with one Cs ion adduct. The charge state of $Au_{24}(S\text{-}tBu)_{16}Cs$ is +1. The experimental isotopic pattern is a match with the simulated isotopic patterns.

Au(core), Au(monomeric)—Au(core), Au(trimeric)—Au(core), Au(core)—S(bridging), Au(trimeric)—S and Au(monomeric)—S bond distances.

The presence of the title nanomolecule, $Au_{24}(S\text{-}tBu)_{16}$, along with $Au_{23}(S\text{-}tBu)_{16}$ and $Au_{25}(S\text{-}tBu)_{16}$, was confirmed by ESI–MS (see Figs. 4 and 5, and Fig. S3 in the supporting information). $Au_{24}(S\text{-}tBu)_{16}$ ionizes in the positive mode with a Cs ion adduct at m/z = 6284.7 Da. Since Cs is needed for the ionization of $Au_{24}(S\text{-}tBu)_{16}$, this suggests that the $Au_{24}(S\text{-}tBu)_{16}$ nanomolecule is neutral. This is further confirmed by the absence of a counter-ion in the X-ray structure. The theoretical spectra of $Au_{24}(S\text{-}tBu)_{16}$ are in agreement with the experimental spectra. Previously identified $Au_{23}(S\text{-}tBu)_{16}$ (Hesari & Workentin, 2014) is also present in the mixture and is ionized in negative mode ESI at 5954.9 Da. The experimental spectra agree well with the theoretical spectra of $Au_{23}(S\text{-}tBu)_{16}$ (Fig. 5). The $Au_{25}(S\text{-}tBu)_{16}$ AuNM is observed in both positive and negative ESI with m/z = 6348.8 Da, and the isotopic pattern is in good agreement between the experimental and theoretical spectra (Fig. 5).

The UV–Vis spectra of the $Au_{24}(S\text{-}tBu)_{16}$ crude shows a peak at 566 nm (Fig. S4 in the supporting information). This observation is consistent with the previously reported $Au_{23}(S\text{-}tBu)_{16}$ crude (Hesari & Workentin, 2014). The IR spectra of the $Au_{24}(S\text{-}tBu)_{16}$ crude and the neat thiol are given in Fig. S5. The IR spectrum of the Au_{24} crude mimics the IR spectrum of the *tert*-butylthiol ligand (Fig. S5). The same trend was observed previously with different Au clusters capped by different thiol ligands (Farrag *et al.*, 2013; Nieto-Ortega & Bürgi, 2018; Brust *et al.*, 1994).

On an additional note, the structures of $Au_{21}(SR)_{15}$ and $Au_{30}(SR)_{18}$, where *SR* is either *tert*-butylthiol or 1-adamantanethiol, have been reported elsewhere (Xiong *et al.*, 2018; Chen *et al.*, 2016; Dass *et al.*, 2016; Higaki *et al.*, 2016) (for more details, see Table S1 in the supporting information). Even though the number of Au atoms and protecting thiol ligands are the same, the atomic structures of $Au_{21}(S\text{-}tBu)_{15}$ and $Au_{21}(S\text{-}Adm)_{15}$ are different from one another. $Au_{21}(S\text{-}tBu)_{15}$ is built on a 10-atom Au core protected by two dimeric staples, one trimeric staple, and one longer $Au_4(SR)_5$ unit (Xiong *et al.*, 2018). $Au_{21}(S\text{-}Adm)_{15}$ has a 10-atom Au core protected by one monomeric staple, one dimeric staple, one longer $Au_8(SR)_9$ unit, and one bridging thiol (Chen *et al.*, 2016). Because of the diversity of the structures, the Au(core)—Au(core) and Au(staples)—Au(core) bonds are longer in $Au_{21}(S\text{-}tBu)_{15}$ (Xiong *et al.*, 2018). The $Au_{30}(S\text{-}tBu)_{18}$ structure has a 22-atom core protected by two monomeric staples, two trimeric staples, and six bridging ligands (Dass *et al.*, 2016). On the other hand, $Au_{30}(S\text{-}Adm)_{18}$ is assembled by an 18-atom core protected by six dimeric staples (Higaki *et al.*, 2016). Unlike $Au_{24}(SR)_{16}$, both $Au_{21}(SR)_{15}$ and $Au_{30}(SR)_{18}$ show contrasting structural differences regardless of the identical number of Au atoms and thiolate ligands (*SR* is either *tert*-butylthiol or 1-adamantanethiol) and the similarity of the environment around the S—Au bonds. These differences in the structures are not only due to the bulkiness of the

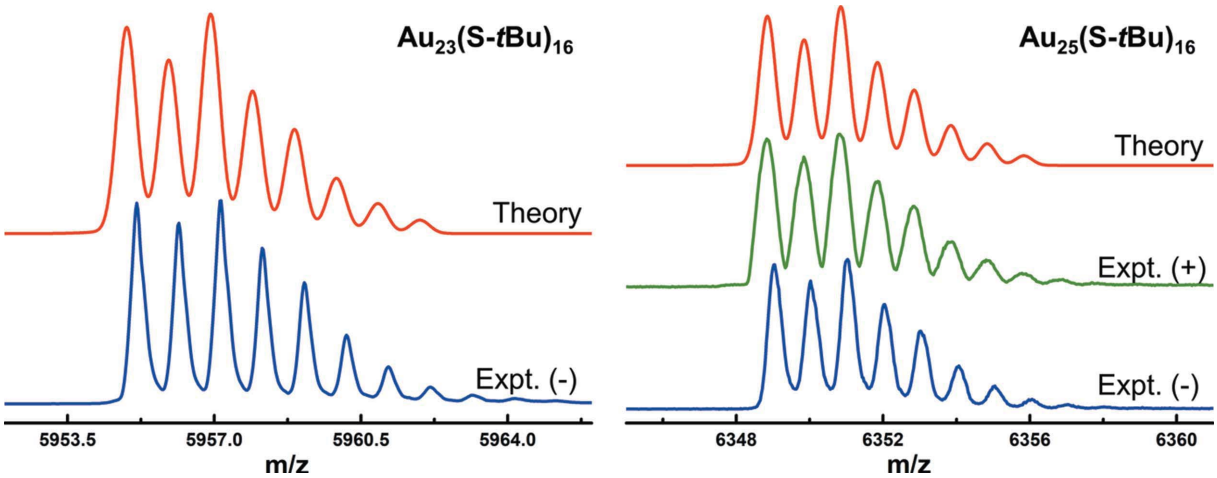

Figure 5
ESI–MS spectra [theoretical (red) and experimental (blue: negative mode, green: positive mode)] for $Au_{23}(S\text{-}tBu)_{16}$ (left) and $Au_{25}(S\text{-}tBu)_{16}$ (right). The experimental isotopic patterns are a match with the simulated isotopic patterns.

ligand, but also to the electronic nature of the ligand structure (Rambukwella *et al.*, 2018). The reason for the similarity of the structures of $Au_{24}(SR)_{16}$ requires further theoretical analysis. Interestingly, the Au_{30} and Au_{24} units protected by *tert*-butylthiol show some similarities in their structures. While Au_{24} has a 13-atom cuboctahedral core, Au_{30} has a 20-atom bicuboctahedral core sharing six Au atoms (Dass *et al.*, 2016). Both these core structures are protected by two monomeric and two trimeric staples.

From a discussion of the Au_{24}(S-Adm)$_{16}$ cluster, Crasto and co-workers proposed the structures of Au_{23}(S-Adm)$_{16}$ and Au_{25}(S-Adm)$_{16}$ based on the Au_{24}(S-Adm)$_{16}$ structure (Crasto, Barcaro *et al.*, 2014). Based on the similarities in these structures, we predict that Au_{23}(S-*t*Bu)$_{16}$ and Au_{25}(S-*t*Bu)$_{16}$ are likely related to Au_{23}(S-Adm)$_{16}$ and Au_{25}(S-Adm)$_{16}$, respectively. Both proposed $Au_{23}(SR)_{16}$ and $Au_{25}(SR)_{16}$ structures have an Au_{13} core protected by two trimeric staples, two monomeric staples, and four bridging thiols. To obtain the Au_{23}(S-*t*Bu)$_{16}$ structure, a symmetrically capping Au atom is removed from the Au_{24}(S-*t*Bu)$_{16}$ structure (Fig. S6). To build the Au_{25}(S-*t*Bu)$_{16}$ structure, an extra capping Au atom is added to the empty (100) square face of the Au_{24}(S-*t*Bu)$_{16}$ core, as shown in Fig. S6. An Au_{23} unit in cyclohexanethiol has an Au_{13} cuboctahedral core with two capping Au atoms protected by two trimeric and two monomeric staples (Das *et al.*, 2013). This structure is in agreement with the proposed $Au_{23}(SR)_{16}$ structures in Au_{23}(S-*t*Bu)$_{16}$ and Au_{23}(S-Adm)$_{16}$.

4. Conclusion

In summary, Au_{24}(S-*t*Bu)$_{16}$ was synthesized and crystallized in the monoclinic space group *Cc*. It is built on a 16-atom core protected by two monomeric staples, two trimeric staples, and four bridging thiol ligands. The Au_{24}(S-*t*Bu)$_{16}$ structure is similar to the 1-adamantanethiol-protected counterpart. ESI–MS shows the presence of the title nanomolecule along with Au_{23}(S-*t*Bu)$_{16}$ and Au_{25}(S-*t*Bu)$_{16}$. Au_{24}(S-*t*Bu)$_{16}$ is neutral as it ionizes in the ESI–MS with a Cs adduct, and this is further confirmed by the absence of a counter-ion in the X-ray crystallography data.

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References

Alvarez, M. M., Khoury, J. T., Schaaff, T. G., Shafigullin, M. N., Vezmar, I. & Whetten, R. L. (1997). *J. Phys. Chem. B*, **101**, 3706–3712.
Boisselier, E. & Astruc, D. (2009). *Chem. Soc. Rev.* **38**, 1759–1782.
Bowman, M.-C., Ballard, T. E., Ackerson, C. J., Feldheim, D. L., Margolis, D. M. & Melander, C. (2008). *J. Am. Chem. Soc.* **130**, 6896–6897.
Brown, S. D., Nativo, P., Smith, J.-A., Stirling, D., Edwards, P. R., Venugopal, B., Flint, D. J., Plumb, J. A., Graham, D. & Wheate, N. J. (2010). *J. Am. Chem. Soc.* **132**, 4678–4684.
Bruker (2014). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2019). *APEX-3* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Brust, M., Walker, M., Bethell, D., Schiffrin, D. J. & Whyman, R. (1994). *J. Chem. Soc. Chem. Commun.* pp. 801–802.
Chaki, N. K., Negishi, Y., Tsunoyama, H., Shichibu, Y. & Tsukuda, T. (2008). *J. Am. Chem. Soc.* **130**, 8608–8610.
Chen, S., Xiong, L., Wang, S., Ma, Z., Jin, S., Sheng, H., Pei, Y. & Zhu, M. (2016). *J. Am. Chem. Soc.* **138**, 10754–10757.
Crasto, D., Barcaro, G., Stener, M., Sementa, L., Fortunelli, A. & Dass, A. (2014). *J. Am. Chem. Soc.* **136**, 14933–14940.
Crasto, D. & Dass, A. (2013). *J. Phys. Chem. C*, **117**, 22094–22097.
Crasto, D., Malola, S., Brosofsky, G., Dass, A. & Häkkinen, H. (2014). *J. Am. Chem. Soc.* **136**, 5000–5005.
Das, A., Li, T., Nobusada, K., Zeng, C., Rosi, N. L. & Jin, R. (2013). *J. Am. Chem. Soc.* **135**, 18264–18267.
Dass, A., Jones, T., Rambukwella, M., Crasto, D., Gagnon, K. J., Sementa, L., De Vetta, M., Baseggio, O., Aprà, E., Stener, M. & Fortunelli, A. (2016). *J. Phys. Chem. C*, **120**, 6256–6261.
Dass, A., Theivendran, S., Nimmala, P. R., Kumara, C., Jupally, V. R., Fortunelli, A., Sementa, L., Barcaro, G., Zuo, X. & Noll, B. C. (2015). *J. Am. Chem. Soc.* **137**, 4610–4613.
Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
Du, Y., Sheng, H., Astruc, D. & Zhu, M. (2019). *Chem. Rev.* **120**, 526–622.
Farrag, M., Tschurl, M., Dass, A. & Heiz, U. (2013). *Phys. Chem. Chem. Phys.* **15**, 12539–12542.
Gan, Z., Chen, J., Wang, J., Wang, C., Li, M.-B., Yao, C., Zhuang, S., Xu, A., Li, L. & Wu, Z. (2017). *Nat. Commun.* **8**, 14739.
Häkkinen, H. & Manninen, M. (1996). *Phys. Rev. Lett.* **76**, 1599–1602.
Heaven, M. W., Dass, A., White, P. S., Holt, K. M. & Murray, R. W. (2008). *J. Am. Chem. Soc.* **130**, 3754–3755.
Hesari, M. & Workentin, M. S. (2014). *J. Mater. Chem. C*, **2**, 3631–3638.
Higaki, T., Liu, C., Zeng, C., Jin, R., Chen, Y., Rosi, N. L. & Jin, R. (2016). *Angew. Chem. Int. Ed.* **55**, 6694–6697.
Jones, T. C., Sumner, L., Ramakrishna, G., Hatshan, M., Abuhagr, A., Chakraborty, S. & Dass, A. (2018). *J. Phys. Chem. C*, **122**, 17726–17737.
Kumara, C. & Dass, A. (2014). *Anal. Chem.* **86**, 4227–4232.
Kumara, C., Zuo, X., Cullen, D. A. & Dass, A. (2014). *ACS Nano*, **8**, 6431–6439.
Levi-Kalisman, Y., Jadzinsky, P. D., Kalisman, N., Tsunoyama, H., Tsukuda, T., Bushnell, D. A. & Kornberg, R. D. (2011). *J. Am. Chem. Soc.* **133**, 2976–2982.
Li, Y., Zhou, M., Song, Y., Higaki, T., Wang, H. & Jin, R. (2021). *Nature*, **594**, 380–384.
Maman, M. P., Nair, A. S., Abdul Hakkim Nazeeja, A. M., Pathak, B. & Mandal, S. (2020). *J. Phys. Chem. Lett.* **11**, 10052–10059.
Murray, R. W. (2008). *Chem. Rev.* **108**, 2688–2720.
Negishi, Y., Nobusada, K. & Tsukuda, T. (2005). *J. Am. Chem. Soc.* **127**, 5261–5270.
Negishi, Y., Sakamoto, C., Ohyama, T. & Tsukuda, T. (2012). *J. Phys. Chem. Lett.* **3**, 1624–1628.
Nieto-Ortega, B. & Bürgi, T. (2018). *Acc. Chem. Res.* **51**, 2811–2819.
Palmer, D. C. (2014). *CrystalMaker*. CrystalMaker Software Ltd, Begbroke, Oxfordshire, England.
Rambukwella, M., Sakthivel, N. A., Delcamp, J. H., Sementa, L., Fortunelli, A. & Dass, A. (2018). *Front. Chem.* **6**, 330.
Riccardi, L., De Biasi, F., De Vivo, M., Bürgi, T., Rastrelli, F. & Salassa, G. (2019). *ACS Nano*, **13**, 7127–7134.

Saha, K., Agasti, S. S., Kim, C., Li, X. & Rotello, V. M. (2012). *Chem. Rev.* **112**, 2739–2779.
Sakthivel, N. A. & Dass, A. (2018). *Acc. Chem. Res.* **51**, 1774–1783.
Sakthivel, N. A., Shabaninezhad, M., Sementa, L., Yoon, B., Stener, M., Whetten, R. L., Ramakrishna, G., Fortunelli, A., Landman, U. & Dass, A. (2020). *J. Am. Chem. Soc.* **142**, 15799–15814.
Sakthivel, N. A., Stener, M., Sementa, L., Fortunelli, A., Ramakrishna, G. & Dass, A. (2018). *J. Phys. Chem. Lett.* **9**, 1295–1300.
Sakthivel, N. A., Theivendran, S., Ganeshraj, V., Oliver, A. G. & Dass, A. (2017). *J. Am. Chem. Soc.* **139**, 15450–15459.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Tlahuice-Flores, A., Whetten, R. L. & Jose-Yacaman, M. (2013). *J. Phys. Chem. C*, **117**, 20867–20875.
Walter, M., Akola, J., Lopez-Acevedo, O., Jadzinsky, P. D., Calero, G., Ackerson, C. J., Whetten, R. L., Grönbeck, H. & Häkkinen, H. (2008). *Proc. Natl Acad. Sci. USA*, **105**, 9157–9162.
Wang, A.-Q., Chang, C.-M. & Mou, C.-Y. (2005). *J. Phys. Chem. B*, **109**, 18860–18867.
Wey, K. & Epple, M. (2020). *J. Mater. Sci. Mater. Med.* **31**, 117.
Wu, Z., Mullins, D. R., Allard, L. F., Zhang, Q. & Wang, L. (2018). *Chin. Chem. Lett.* **29**, 795–799.
Xiong, L., Yang, S., Sun, X., Chai, J., Rao, B., Yi, L., Zhu, M. & Pei, Y. (2018). *J. Phys. Chem. C*, **122**, 14898–14907.
Yan, N., Xia, N., Liao, L., Zhu, M., Jin, F., Jin, R. & Wu, Z. (2018). *Sci. Adv.* **4**, eaat7259.
Yang, H., Wang, Y., Edwards, A. J., Yan, J. & Zheng, N. (2014). *Chem. Commun.* **50**, 14325–14327.

supporting information

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Crystal structure of bulky-ligand-protected $Au_{24}(S\text{-}C_4H_9)_{16}$

Kalpani Hirunika Wijesinghe, Allen G. Oliver and Amala Dass

Computing details

Data collection: *APEX3* (Bruker, 2019); cell refinement: *SAINT* (Bruker, 2019); data reduction: *SAINT* (Bruker, 2019); program(s) used to solve structure: SHELXT2018 (Sheldrick, 2015*a*); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015*b*); molecular graphics: OLEX2 (Dolomanov *et al.*, 2009) and *CrystalMaker* (Palmer, 2014); software used to prepare material for publication: OLEX2 (Dolomanov *et al.*, 2009).

Poly[hexadecakis(*μ*-*tert*-butylthiolato)tetracosagold]

Crystal data

$[Au_{24}(C_4H_9S)_{16}]$
M_r = 6153.94
Monoclinic, *Cc*
a = 15.5946 (6) Å
b = 25.9193 (6) Å
c = 29.7621 (8) Å
β = 100.655 (2)°
V = 11822.5 (6) Å^3
Z = 4
F(000) = 10720
D_x = 3.457 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.54178 Å
Cell parameters from 9932 reflections
θ = 3.0–70.3°
μ = 57.21 mm^{-1}
T = 120 K
Blade, metallic dark brown
0.08 × 0.04 × 0.02 mm

Data collection

Bruker PHOTON-II CMOS diffractometer
Detector resolution: 7.41 pixels mm^{-1}
φ and *ω* scans
Absorption correction: multi-scan (SADABS2014; Bruker, 2014)
T_{min} = 0.362, T_{max} = 0.753
57304 measured reflections
21231 independent reflections
19685 reflections with $I > 2\sigma(I)$
R_{int} = 0.074
θ_{max} = 70.5°, θ_{min} = 3.0°
h = −18→18
k = −31→31
l = −35→36

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.121
S = 1.00
21231 reflections
986 parameters
26 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.069P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.010
$\Delta\rho_{max}$ = 3.09 e Å^{-3}
$\Delta\rho_{min}$ = −2.63 e Å^{-3}
Absolute structure: Refined as an inversion twin.
Absolute structure parameter: 0.42 (2)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refined as a 2-component inversion twin.
Throughout the data collection, the crystal was kept below 120 K. The structure was modeled in *OLEX2* (Dolomanov *et al.*, 2009) and solved by SHELXT using Intrinsic Phasing methods (Sheldrick, 2015*a*) and refined by full-matrix least-squares analysis (Sheldrick, 2015*b*). All the non-H atoms were refined using anisotropic displacement parameters.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Au1	0.48656 (7)	0.39408 (4)	0.48381 (3)	0.0270 (2)
Au2	0.63701 (7)	0.35358 (4)	0.54737 (3)	0.0300 (2)
Au3	0.68088 (7)	0.44516 (4)	0.51519 (3)	0.0288 (2)
Au4	0.34676 (7)	0.44264 (4)	0.51240 (3)	0.0295 (2)
Au5	0.62699 (7)	0.35197 (4)	0.44863 (3)	0.0303 (2)
Au6	0.46906 (7)	0.38877 (4)	0.57375 (3)	0.0316 (2)
Au7	0.51448 (7)	0.47869 (4)	0.53718 (4)	0.0322 (2)
Au8	0.48267 (7)	0.39670 (4)	0.39177 (3)	0.0317 (2)
Au9	0.33519 (7)	0.44164 (4)	0.41360 (3)	0.0306 (2)
Au10	0.44719 (7)	0.28862 (4)	0.52848 (4)	0.0324 (2)
Au11	0.15871 (7)	0.43636 (4)	0.43341 (4)	0.0337 (2)
Au12	0.30058 (7)	0.34698 (4)	0.44428 (4)	0.0309 (2)
Au13	0.46782 (7)	0.30463 (4)	0.43278 (4)	0.0335 (2)
Au14	0.52263 (7)	0.50266 (4)	0.43415 (4)	0.0317 (2)
Au15	0.69043 (7)	0.43254 (4)	0.60389 (3)	0.0328 (2)
Au16	0.31547 (8)	0.35753 (4)	0.35777 (4)	0.0337 (2)
Au17	0.64687 (7)	0.42724 (4)	0.37638 (3)	0.0334 (2)
Au18	0.86223 (8)	0.45830 (5)	0.58461 (4)	0.0366 (2)
Au19	0.13455 (8)	0.33778 (4)	0.36547 (4)	0.0366 (2)
Au20	0.69865 (8)	0.54454 (4)	0.57753 (4)	0.0370 (2)
Au21	0.82084 (8)	0.35953 (4)	0.52016 (4)	0.0361 (2)
Au22	0.47777 (8)	0.36298 (5)	0.30111 (4)	0.0395 (3)
Au23	0.57686 (8)	0.40599 (5)	0.66969 (4)	0.0388 (3)
Au24	0.28957 (8)	0.24427 (5)	0.37934 (5)	0.0435 (3)
S1	0.3792 (5)	0.5288 (2)	0.4256 (2)	0.0342 (13)
S2	0.1957 (4)	0.4502 (3)	0.5108 (2)	0.0337 (13)
S3	0.3025 (4)	0.3149 (3)	0.5186 (2)	0.0332 (13)
S4	0.6675 (4)	0.4812 (2)	0.43970 (19)	0.0296 (12)
S5	0.5930 (5)	0.2664 (2)	0.5378 (2)	0.0353 (13)
S6	0.6244 (5)	0.3809 (3)	0.3095 (2)	0.0402 (15)
S7	0.1151 (5)	0.4257 (3)	0.3548 (2)	0.0362 (13)
S8	0.4457 (5)	0.3652 (3)	0.6473 (2)	0.0372 (14)
S9	0.1404 (5)	0.2500 (3)	0.3750 (3)	0.0412 (15)
S10	0.8450 (5)	0.5459 (3)	0.5722 (3)	0.0397 (14)
S11	0.5559 (5)	0.5487 (3)	0.5874 (2)	0.0376 (14)

S12	0.7770 (5)	0.3453 (3)	0.4425 (2)	0.0355 (13)
S13	0.3348 (5)	0.3370 (3)	0.2827 (2)	0.0421 (15)
S14	0.8808 (4)	0.3707 (3)	0.5965 (2)	0.0374 (14)
S15	0.4377 (5)	0.2355 (3)	0.3803 (3)	0.0443 (16)
S16	0.7079 (5)	0.4483 (3)	0.6838 (2)	0.0434 (16)
C1	0.714 (2)	0.5830 (11)	0.4569 (11)	0.043 (7)
H1A	0.652242	0.590500	0.446595	0.064*
H1B	0.749033	0.612851	0.450662	0.064*
H1C	0.725665	0.575910	0.489769	0.064*
C2	0.740 (2)	0.5351 (10)	0.4308 (9)	0.035 (6)
C3	0.380 (2)	0.4677 (15)	0.6534 (15)	0.063 (11)
H3A	0.329150	0.487604	0.657552	0.095*
H3B	0.389933	0.471823	0.621935	0.095*
H3C	0.431850	0.480110	0.674713	0.095*
C4	0.196 (2)	0.5293 (12)	0.5694 (9)	0.039 (6)
H4A	0.187557	0.565961	0.575526	0.059*
H4B	0.258010	0.520716	0.577603	0.059*
H4C	0.162853	0.508362	0.587737	0.059*
C5	0.534 (3)	0.6254 (15)	0.5204 (17)	0.073 (12)
H5A	0.597285	0.630157	0.524461	0.110*
H5B	0.504484	0.657485	0.509040	0.110*
H5C	0.515870	0.597609	0.498401	0.110*
C6	0.784 (2)	0.4059 (12)	0.7190 (9)	0.043 (7)
C7	0.8309 (19)	0.5198 (10)	0.4464 (10)	0.036 (6)
H7A	0.837394	0.504480	0.476945	0.054*
H7B	0.868696	0.550103	0.447530	0.054*
H7C	0.847415	0.494352	0.425125	0.054*
C8	0.7320 (19)	0.2423 (14)	0.6059 (12)	0.048 (8)
H8A	0.761273	0.214509	0.592254	0.072*
H8B	0.751724	0.242233	0.639122	0.072*
H8C	0.746257	0.275537	0.593402	0.072*
C9	0.630 (2)	0.2336 (11)	0.5944 (11)	0.043 (7)
C10	0.885 (3)	0.6359 (13)	0.6168 (13)	0.055 (9)
H10A	0.916744	0.648639	0.593640	0.083*
H10B	0.902982	0.655062	0.645314	0.083*
H10C	0.821940	0.640760	0.605925	0.083*
C11	0.511 (2)	0.6119 (14)	0.5644 (16)	0.057 (9)
C12	0.545 (3)	0.6507 (12)	0.5982 (13)	0.065 (11)
H12A	0.515308	0.647983	0.624378	0.097*
H12B	0.535219	0.685065	0.584554	0.097*
H12C	0.607721	0.645063	0.608425	0.097*
C13	0.196 (3)	0.5536 (12)	0.4877 (12)	0.052 (9)
H13A	0.176293	0.541931	0.456136	0.078*
H13B	0.260008	0.554160	0.494571	0.078*
H13C	0.173670	0.588400	0.491263	0.078*
C14	−0.005 (2)	0.4378 (13)	0.3394 (13)	0.051 (8)
C15	1.005 (2)	0.2978 (15)	0.5985 (17)	0.065 (11)
H15A	0.986871	0.281014	0.624790	0.098*

H15B	1.064308	0.286975	0.596595	0.098*
H15C	0.964963	0.287773	0.570424	0.098*
C16	1.0024 (18)	0.3563 (13)	0.6043 (10)	0.042 (7)
C17	0.311 (3)	0.384 (2)	0.1982 (12)	0.077 (14)
H17A	0.285440	0.412804	0.178961	0.115*
H17B	0.293684	0.351319	0.182224	0.115*
H17C	0.374271	0.386865	0.204555	0.115*
C18	0.239 (2)	0.2521 (10)	0.5739 (11)	0.041 (7)
H18A	0.200378	0.276606	0.585297	0.062*
H18B	0.299659	0.258941	0.588513	0.062*
H18C	0.223296	0.216829	0.581040	0.062*
C19	0.758 (3)	0.406 (2)	0.7669 (12)	0.073 (13)
H19A	0.785615	0.435855	0.784485	0.110*
H19B	0.778077	0.374278	0.783114	0.110*
H19C	0.694696	0.408960	0.763397	0.110*
C20	0.164 (2)	0.5183 (12)	0.5190 (11)	0.044 (7)
C21	0.381 (3)	0.6205 (15)	0.3829 (16)	0.067 (9)
H21A	0.379130	0.640433	0.354743	0.101*
H21B	0.440507	0.621763	0.401038	0.101*
H21C	0.340174	0.635108	0.400642	0.101*
C22	0.779 (2)	0.2413 (13)	0.4660 (10)	0.047 (8)
H22A	0.808647	0.251069	0.496710	0.071*
H22B	0.795829	0.206135	0.459186	0.071*
H22C	0.715582	0.242710	0.464419	0.071*
C23	0.368 (2)	0.4057 (19)	0.7162 (12)	0.065 (12)
H23A	0.338334	0.435791	0.726356	0.098*
H23B	0.428385	0.404684	0.732407	0.098*
H23C	0.337618	0.374168	0.722965	0.098*
C24	0.3654 (16)	0.4094 (13)	0.6629 (11)	0.041 (7)
C25	0.095 (3)	0.1610 (14)	0.323 (2)	0.080 (15)
H25A	0.050749	0.144011	0.300429	0.120*
H25B	0.088274	0.150219	0.353951	0.120*
H25C	0.153342	0.151176	0.318208	0.120*
C26	0.125 (3)	0.2370 (15)	0.2815 (14)	0.071 (12)
H26A	0.185094	0.223494	0.285331	0.107*
H26B	0.127176	0.274815	0.281761	0.107*
H26C	0.091672	0.225031	0.252296	0.107*
C27	0.879 (2)	0.4254 (18)	0.7218 (12)	0.060 (10)
H27A	0.896244	0.420735	0.692162	0.091*
H27B	0.917869	0.405874	0.745245	0.091*
H27C	0.881467	0.462128	0.729895	0.091*
C28	0.138 (2)	0.2740 (12)	0.5031 (13)	0.048 (8)
H28A	0.136421	0.283870	0.471090	0.072*
H28B	0.120872	0.303524	0.519925	0.072*
H28C	0.098206	0.245223	0.504418	0.072*
C29	0.278 (3)	0.3848 (17)	0.2415 (11)	0.061 (10)
C30	0.611 (2)	0.1772 (16)	0.5875 (15)	0.068 (12)
H30A	0.547450	0.171867	0.580201	0.102*

H30B	0.635080	0.158359	0.615462	0.102*
H30C	0.637199	0.164483	0.562173	0.102*
C31	0.603 (2)	0.3993 (19)	0.2164 (11)	0.063 (11)
H31A	0.643766	0.370466	0.215607	0.094*
H31B	0.605932	0.422637	0.190789	0.094*
H31C	0.543893	0.385964	0.213945	0.094*
C32	0.291 (3)	0.4407 (12)	0.2617 (14)	0.062 (10)
H32A	0.299081	0.464765	0.237456	0.093*
H32B	0.342291	0.441388	0.286158	0.093*
H32C	0.239171	0.450770	0.273972	0.093*
C34	0.578 (2)	0.4773 (15)	0.2654 (14)	0.058 (9)
H34A	0.516609	0.472013	0.250825	0.087*
H34B	0.602310	0.505769	0.250209	0.087*
H34C	0.580862	0.485624	0.297745	0.087*
C33	0.776 (2)	0.3492 (12)	0.7015 (13)	0.051 (8)
H33A	0.714499	0.339642	0.693765	0.076*
H33B	0.806222	0.326201	0.725529	0.076*
H33C	0.802976	0.346079	0.674334	0.076*
C35	0.588 (3)	0.2577 (19)	0.6311 (13)	0.073 (13)
H35A	0.591898	0.295363	0.629423	0.109*
H35B	0.617660	0.245855	0.661181	0.109*
H35C	0.526106	0.247581	0.626497	0.109*
C36	0.725 (2)	0.4417 (15)	0.2671 (12)	0.056 (10)
H36A	0.747539	0.451508	0.298940	0.084*
H36B	0.733295	0.470466	0.246915	0.084*
H36C	0.757787	0.411552	0.259280	0.084*
C37	0.085 (3)	0.2187 (14)	0.3189 (17)	0.066 (11)
C38	−0.015 (3)	0.4978 (14)	0.3480 (13)	0.060 (9)
H38A	0.020208	0.507277	0.377569	0.090*
H38B	−0.076736	0.505727	0.348241	0.090*
H38C	0.004146	0.517369	0.323614	0.090*
C39	0.475 (2)	0.1748 (15)	0.4064 (15)	0.059 (9)
C40	0.804 (2)	0.2775 (11)	0.4321 (10)	0.039 (6)
C41	0.276 (3)	0.3928 (17)	0.6382 (12)	0.062 (10)
H41A	0.266434	0.356543	0.645303	0.093*
H41B	0.272602	0.396638	0.605134	0.093*
H41C	0.231391	0.414269	0.648100	0.093*
C42	0.995 (3)	0.5676 (18)	0.6288 (17)	0.077 (14)
H42A	1.004088	0.530243	0.628248	0.115*
H42B	1.027415	0.581758	0.657605	0.115*
H42C	1.016420	0.583566	0.603091	0.115*
C43	0.577 (3)	0.1744 (17)	0.417 (2)	0.087 (15)
H43A	0.599467	0.160970	0.390961	0.130*
H43B	0.597446	0.152444	0.444011	0.130*
H43C	0.598773	0.209665	0.423952	0.130*
C44	0.759 (3)	0.2640 (14)	0.3864 (12)	0.056 (9)
H44A	0.799314	0.245118	0.370598	0.084*
H44B	0.739679	0.295527	0.369414	0.084*

H44C	0.708709	0.242258	0.388434	0.084*
C45	0.260 (3)	0.2103 (12)	0.5022 (14)	0.056 (9)
H45A	0.218567	0.182172	0.503381	0.084*
H45B	0.317901	0.200093	0.518600	0.084*
H45C	0.262986	0.217869	0.470245	0.084*
C46	0.066 (2)	0.5194 (13)	0.5101 (10)	0.045 (7)
H46A	0.043687	0.485495	0.517146	0.067*
H46B	0.044091	0.527666	0.477911	0.067*
H46C	0.045777	0.545624	0.529513	0.067*
C47	0.905 (3)	0.2756 (16)	0.4347 (16)	0.068 (11)
H47A	0.934541	0.280591	0.466479	0.102*
H47B	0.922511	0.302988	0.415590	0.102*
H47C	0.921475	0.241989	0.423791	0.102*
C48	0.444 (3)	0.1320 (11)	0.3708 (14)	0.057 (9)
H48A	0.398233	0.145426	0.346806	0.085*
H48B	0.421878	0.102610	0.385876	0.085*
H48C	0.493878	0.120685	0.357230	0.085*
C49	0.872 (3)	0.5599 (17)	0.6666 (10)	0.063 (11)
H49A	0.808662	0.555178	0.659234	0.094*
H49B	0.886456	0.585390	0.691149	0.094*
H49C	0.900068	0.526959	0.676569	0.094*
C50	1.041 (3)	0.3817 (14)	0.5685 (14)	0.058 (9)
H50A	1.020701	0.364517	0.539179	0.086*
H50B	1.104735	0.379547	0.576431	0.086*
H50C	1.023193	0.418025	0.566219	0.086*
C51	0.629 (2)	0.4284 (12)	0.2612 (10)	0.042 (7)
C52	−0.0273 (19)	0.4280 (16)	0.2880 (11)	0.053 (9)
H52A	−0.036491	0.461077	0.271850	0.080*
H52B	−0.080492	0.407209	0.280896	0.080*
H52C	0.021031	0.409557	0.278317	0.080*
C53	0.230 (2)	0.2578 (11)	0.5243 (10)	0.039 (7)
C54	1.040 (3)	0.3729 (19)	0.6536 (10)	0.070 (13)
H54A	1.005805	0.401969	0.662054	0.105*
H54B	1.100783	0.383476	0.655766	0.105*
H54C	1.036652	0.343965	0.674387	0.105*
C55	−0.006 (2)	0.232 (2)	0.3154 (18)	0.083 (15)
H55A	−0.038802	0.219054	0.286434	0.124*
H55B	−0.011478	0.269555	0.316631	0.124*
H55C	−0.028116	0.216340	0.340905	0.124*
C56	−0.055 (2)	0.4076 (17)	0.3673 (13)	0.061 (11)
H56A	−0.030950	0.372618	0.371494	0.091*
H56B	−0.116282	0.405736	0.351886	0.091*
H56C	−0.051580	0.424103	0.397210	0.091*
C57	0.904 (3)	0.5784 (16)	0.6252 (15)	0.061 (9)
C58	0.188 (3)	0.368 (2)	0.2337 (13)	0.080 (15)
H58A	0.176246	0.349845	0.260825	0.120*
H58B	0.177057	0.344609	0.207328	0.120*
H58C	0.149321	0.398003	0.227555	0.120*

C59	0.253 (2)	0.5625 (18)	0.3556 (15)	0.069 (10)
H59A	0.224689	0.584227	0.375668	0.104*
H59B	0.233935	0.526668	0.357700	0.104*
H59C	0.235942	0.574555	0.323968	0.104*
C60	0.437 (2)	0.1631 (14)	0.4508 (12)	0.053 (8)
H60A	0.470807	0.181888	0.476697	0.080*
H60B	0.440553	0.125971	0.457117	0.080*
H60C	0.375774	0.174110	0.446262	0.080*
C61	0.357 (2)	0.5661 (13)	0.3712 (12)	0.049 (5)
C62	0.404 (3)	0.6057 (19)	0.559 (2)	0.084 (15)
H62A	0.381628	0.584341	0.532422	0.127*
H62B	0.376642	0.639816	0.555405	0.127*
H62C	0.390539	0.589194	0.586693	0.127*
C63	0.395 (3)	0.5435 (19)	0.3357 (16)	0.075 (10)
H63A	0.404626	0.570212	0.313825	0.113*
H63B	0.356292	0.516918	0.319995	0.113*
H63C	0.451573	0.527803	0.349079	0.113*
C64	0.722 (2)	0.5497 (10)	0.3794 (8)	0.035 (6)
H64A	0.738792	0.521009	0.361478	0.052*
H64B	0.755350	0.580499	0.374680	0.052*
H64C	0.659314	0.556733	0.369539	0.052*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au1	0.0311 (5)	0.0270 (4)	0.0217 (4)	0.0039 (4)	0.0015 (4)	−0.0005 (3)
Au2	0.0347 (5)	0.0296 (5)	0.0240 (5)	0.0029 (4)	0.0010 (4)	0.0029 (4)
Au3	0.0345 (5)	0.0285 (5)	0.0230 (5)	0.0024 (4)	0.0039 (4)	0.0018 (4)
Au4	0.0314 (5)	0.0309 (5)	0.0250 (5)	0.0050 (4)	0.0022 (4)	0.0015 (4)
Au5	0.0329 (5)	0.0321 (5)	0.0251 (5)	0.0045 (4)	0.0028 (4)	0.0018 (4)
Au6	0.0385 (6)	0.0322 (5)	0.0229 (5)	0.0043 (4)	0.0023 (4)	0.0017 (4)
Au7	0.0358 (6)	0.0300 (5)	0.0301 (5)	0.0004 (4)	0.0044 (4)	−0.0043 (4)
Au8	0.0348 (5)	0.0367 (5)	0.0219 (5)	0.0041 (4)	0.0007 (4)	0.0012 (4)
Au9	0.0341 (5)	0.0295 (5)	0.0268 (5)	0.0030 (4)	0.0023 (4)	0.0020 (4)
Au10	0.0368 (6)	0.0289 (5)	0.0305 (5)	0.0006 (4)	0.0033 (4)	0.0016 (4)
Au11	0.0341 (6)	0.0344 (5)	0.0308 (5)	0.0032 (5)	0.0012 (4)	−0.0016 (4)
Au12	0.0344 (5)	0.0295 (5)	0.0278 (5)	0.0033 (4)	0.0028 (4)	0.0020 (4)
Au13	0.0378 (6)	0.0284 (5)	0.0328 (5)	0.0015 (4)	0.0027 (4)	−0.0041 (4)
Au14	0.0353 (5)	0.0312 (5)	0.0277 (5)	0.0008 (4)	0.0033 (4)	0.0015 (4)
Au15	0.0385 (6)	0.0374 (5)	0.0220 (5)	0.0009 (5)	0.0045 (4)	−0.0008 (4)
Au16	0.0359 (6)	0.0381 (5)	0.0250 (5)	0.0010 (5)	−0.0001 (4)	−0.0027 (4)
Au17	0.0383 (6)	0.0384 (5)	0.0227 (5)	0.0014 (5)	0.0034 (4)	0.0014 (4)
Au18	0.0374 (6)	0.0379 (6)	0.0340 (5)	0.0032 (5)	0.0049 (4)	−0.0020 (4)
Au19	0.0367 (6)	0.0329 (5)	0.0383 (6)	0.0039 (5)	0.0024 (5)	−0.0030 (4)
Au20	0.0393 (6)	0.0333 (5)	0.0365 (6)	0.0024 (5)	0.0019 (5)	−0.0034 (4)
Au21	0.0357 (6)	0.0350 (5)	0.0368 (6)	0.0032 (5)	0.0044 (5)	−0.0006 (4)
Au22	0.0468 (7)	0.0455 (6)	0.0257 (5)	−0.0027 (5)	0.0053 (5)	−0.0039 (4)
Au23	0.0383 (6)	0.0512 (7)	0.0256 (5)	0.0034 (5)	0.0022 (4)	0.0005 (4)

Au24	0.0420 (7)	0.0353 (6)	0.0484 (7)	0.0069 (5)	−0.0044 (5)	−0.0066 (5)
S1	0.039 (3)	0.029 (3)	0.035 (3)	0.007 (3)	0.007 (3)	0.005 (2)
S2	0.032 (3)	0.037 (3)	0.032 (3)	0.003 (3)	0.004 (2)	−0.003 (2)
S3	0.035 (3)	0.035 (3)	0.029 (3)	−0.003 (3)	0.005 (2)	0.003 (2)
S4	0.035 (3)	0.030 (3)	0.023 (3)	0.000 (3)	0.003 (2)	0.003 (2)
S5	0.038 (3)	0.031 (3)	0.036 (3)	0.001 (3)	0.004 (3)	−0.002 (2)
S6	0.045 (4)	0.047 (4)	0.027 (3)	0.006 (3)	0.005 (3)	−0.001 (3)
S7	0.039 (3)	0.034 (3)	0.033 (3)	0.000 (3)	0.000 (3)	−0.001 (2)
S8	0.042 (4)	0.046 (4)	0.024 (3)	0.006 (3)	0.007 (3)	0.005 (2)
S9	0.040 (4)	0.036 (3)	0.046 (4)	0.000 (3)	0.005 (3)	−0.001 (3)
S10	0.038 (4)	0.038 (3)	0.041 (4)	0.003 (3)	0.001 (3)	−0.001 (3)
S11	0.045 (4)	0.032 (3)	0.036 (3)	0.000 (3)	0.007 (3)	−0.005 (2)
S12	0.036 (3)	0.034 (3)	0.036 (3)	0.005 (3)	0.006 (3)	−0.001 (2)
S13	0.052 (4)	0.051 (4)	0.023 (3)	−0.004 (3)	0.005 (3)	−0.007 (3)
S14	0.032 (3)	0.043 (3)	0.035 (3)	0.000 (3)	0.001 (3)	0.000 (3)
S15	0.047 (4)	0.043 (4)	0.040 (4)	0.002 (3)	−0.002 (3)	−0.009 (3)
S16	0.051 (4)	0.057 (4)	0.021 (3)	0.002 (3)	0.003 (3)	−0.005 (3)
C1	0.054 (18)	0.031 (13)	0.042 (15)	−0.002 (13)	0.003 (13)	−0.018 (11)
C2	0.044 (15)	0.028 (12)	0.033 (13)	−0.012 (12)	0.010 (11)	−0.008 (10)
C3	0.05 (2)	0.06 (2)	0.07 (3)	0.005 (17)	−0.006 (18)	−0.034 (19)
C4	0.050 (17)	0.043 (15)	0.025 (13)	−0.002 (13)	0.008 (12)	−0.013 (11)
C5	0.08 (3)	0.037 (17)	0.11 (4)	0.020 (19)	0.03 (3)	−0.002 (19)
C6	0.044 (16)	0.050 (17)	0.023 (13)	0.001 (13)	−0.022 (11)	0.001 (11)
C7	0.044 (15)	0.021 (11)	0.044 (14)	0.005 (11)	0.008 (12)	−0.006 (10)
C8	0.030 (15)	0.06 (2)	0.053 (18)	0.004 (14)	0.010 (13)	0.013 (15)
C9	0.047 (17)	0.028 (13)	0.048 (16)	0.018 (13)	−0.007 (13)	0.001 (11)
C10	0.06 (2)	0.041 (17)	0.05 (2)	−0.009 (16)	−0.015 (16)	−0.006 (14)
C11	0.029 (15)	0.047 (19)	0.09 (3)	0.022 (14)	0.009 (16)	0.012 (18)
C12	0.11 (3)	0.029 (15)	0.05 (2)	0.023 (19)	0.00 (2)	−0.014 (14)
C13	0.08 (2)	0.039 (16)	0.048 (18)	0.021 (16)	0.032 (17)	0.028 (14)
C14	0.051 (19)	0.046 (18)	0.052 (19)	0.012 (15)	0.000 (15)	−0.006 (14)
C15	0.041 (19)	0.05 (2)	0.10 (3)	0.015 (16)	−0.008 (19)	0.011 (19)
C16	0.027 (13)	0.06 (2)	0.031 (15)	0.009 (13)	−0.005 (11)	−0.008 (12)
C17	0.08 (3)	0.12 (4)	0.024 (16)	−0.04 (3)	0.005 (17)	−0.007 (18)
C18	0.056 (18)	0.021 (12)	0.050 (17)	−0.002 (12)	0.019 (14)	0.003 (11)
C19	0.05 (2)	0.14 (4)	0.032 (17)	0.00 (2)	0.002 (15)	−0.01 (2)
C20	0.047 (17)	0.041 (16)	0.041 (16)	0.022 (14)	0.000 (13)	−0.008 (12)
C21	0.07 (2)	0.048 (17)	0.08 (2)	0.004 (16)	0.012 (17)	0.026 (15)
C22	0.053 (18)	0.056 (19)	0.031 (14)	0.020 (16)	0.002 (13)	−0.012 (12)
C23	0.049 (19)	0.12 (3)	0.038 (17)	0.04 (2)	0.025 (15)	0.014 (18)
C24	0.011 (11)	0.062 (19)	0.050 (17)	0.011 (12)	0.008 (10)	−0.023 (14)
C25	0.10 (3)	0.033 (18)	0.12 (4)	−0.01 (2)	0.06 (3)	−0.02 (2)
C26	0.10 (3)	0.05 (2)	0.05 (2)	−0.02 (2)	−0.02 (2)	0.003 (16)
C27	0.048 (19)	0.10 (3)	0.039 (17)	−0.002 (19)	0.010 (14)	−0.011 (17)
C28	0.034 (15)	0.038 (15)	0.08 (2)	−0.001 (13)	0.028 (15)	0.013 (15)
C29	0.07 (2)	0.08 (3)	0.024 (15)	−0.01 (2)	−0.011 (15)	−0.002 (14)
C30	0.06 (2)	0.07 (2)	0.08 (3)	0.027 (19)	0.012 (19)	0.06 (2)
C31	0.049 (19)	0.11 (3)	0.024 (15)	0.00 (2)	−0.012 (13)	−0.001 (16)

C32	0.08 (3)	0.033 (16)	0.07 (2)	0.024 (17)	0.01 (2)	0.027 (15)
C34	0.048 (19)	0.06 (2)	0.06 (2)	−0.003 (17)	−0.007 (16)	0.003 (16)
C33	0.048 (18)	0.037 (16)	0.07 (2)	−0.006 (14)	0.010 (16)	−0.003 (14)
C35	0.07 (3)	0.11 (3)	0.05 (2)	0.02 (2)	0.05 (2)	0.04 (2)
C36	0.05 (2)	0.08 (2)	0.042 (17)	−0.009 (18)	0.018 (15)	0.039 (16)
C37	0.07 (2)	0.035 (17)	0.10 (3)	0.015 (17)	0.03 (2)	−0.022 (18)
C38	0.08 (3)	0.045 (19)	0.06 (2)	0.009 (18)	0.001 (18)	0.003 (15)
C39	0.039 (17)	0.06 (2)	0.08 (3)	0.014 (16)	−0.003 (17)	−0.009 (18)
C40	0.052 (17)	0.025 (12)	0.040 (15)	0.006 (13)	0.008 (13)	−0.013 (10)
C41	0.07 (2)	0.08 (3)	0.033 (17)	−0.01 (2)	0.008 (16)	0.010 (16)
C42	0.05 (2)	0.07 (3)	0.09 (3)	−0.014 (19)	−0.04 (2)	0.00 (2)
C43	0.09 (3)	0.05 (2)	0.11 (4)	0.03 (2)	0.00 (3)	0.01 (2)
C44	0.07 (2)	0.048 (18)	0.047 (18)	0.011 (18)	0.009 (17)	0.002 (14)
C45	0.06 (2)	0.029 (15)	0.07 (2)	0.001 (15)	0.009 (19)	−0.008 (15)
C46	0.042 (16)	0.054 (18)	0.036 (14)	0.029 (15)	0.003 (12)	−0.006 (12)
C47	0.06 (2)	0.06 (2)	0.09 (3)	0.04 (2)	0.02 (2)	0.02 (2)
C48	0.08 (3)	0.021 (13)	0.08 (2)	−0.014 (15)	0.03 (2)	−0.019 (14)
C49	0.07 (2)	0.09 (3)	0.018 (13)	−0.03 (2)	−0.007 (14)	0.007 (14)
C50	0.06 (2)	0.050 (19)	0.06 (2)	0.008 (18)	0.030 (19)	0.002 (16)
C51	0.049 (17)	0.041 (15)	0.038 (15)	0.002 (14)	0.013 (13)	−0.020 (12)
C52	0.023 (13)	0.09 (3)	0.047 (17)	0.032 (16)	0.000 (12)	−0.023 (16)
C53	0.050 (17)	0.041 (15)	0.034 (14)	−0.016 (13)	0.029 (13)	−0.023 (11)
C54	0.07 (2)	0.11 (3)	0.018 (14)	0.04 (2)	−0.010 (14)	−0.014 (16)
C55	0.037 (19)	0.11 (4)	0.09 (3)	−0.01 (2)	−0.01 (2)	−0.03 (3)
C56	0.031 (15)	0.09 (3)	0.06 (2)	0.030 (18)	0.025 (15)	0.03 (2)
C57	0.06 (2)	0.06 (2)	0.07 (2)	0.020 (18)	0.004 (18)	−0.003 (17)
C58	0.05 (2)	0.16 (5)	0.034 (18)	−0.02 (3)	−0.001 (15)	0.00 (2)
C59	0.050 (17)	0.08 (2)	0.066 (19)	0.005 (16)	−0.019 (15)	0.039 (16)
C60	0.06 (2)	0.048 (18)	0.044 (18)	0.011 (16)	−0.005 (15)	−0.009 (14)
C61	0.050 (10)	0.042 (10)	0.052 (10)	0.015 (9)	0.000 (9)	0.014 (9)
C62	0.09 (3)	0.07 (3)	0.10 (4)	0.02 (3)	0.04 (3)	0.01 (3)
C63	0.08 (2)	0.07 (2)	0.064 (19)	0.011 (19)	−0.002 (18)	0.013 (17)
C64	0.059 (18)	0.036 (13)	0.011 (10)	−0.002 (13)	0.012 (11)	0.008 (9)

Geometric parameters (Å, º)

Au1—Au2	2.9230 (15)	C13—H13A	0.9800
Au1—Au3	3.2804 (15)	C13—H13B	0.9800
Au1—Au4	2.7834 (15)	C13—H13C	0.9800
Au1—Au5	2.8164 (15)	C13—C20	1.46 (4)
Au1—Au6	2.7438 (14)	C14—C38	1.59 (5)
Au1—Au7	2.6957 (15)	C14—C52	1.53 (5)
Au1—Au8	2.7297 (14)	C14—C56	1.47 (5)
Au1—Au9	3.1040 (14)	C15—H15A	0.9800
Au1—Au10	3.1493 (15)	C15—H15B	0.9800
Au1—Au12	3.1661 (15)	C15—H15C	0.9800
Au1—Au13	2.7575 (15)	C15—C16	1.53 (5)
Au1—Au14	3.2756 (15)	C16—C50	1.47 (5)

Au2—Au3	2.6947 (15)	C16—C54	1.54 (4)
Au2—Au5	2.9143 (14)	C17—H17A	0.9800
Au2—Au6	3.0114 (16)	C17—H17B	0.9800
Au2—Au10	3.3614 (16)	C17—H17C	0.9800
Au2—Au15	2.6822 (15)	C17—C29	1.47 (5)
Au2—Au21	3.1235 (17)	C18—H18A	0.9800
Au2—S5	2.363 (7)	C18—H18B	0.9800
Au3—Au5	3.1383 (15)	C18—H18C	0.9800
Au3—Au7	2.9233 (15)	C18—C53	1.46 (4)
Au3—Au15	2.6370 (14)	C19—H19A	0.9800
Au3—Au18	3.1972 (16)	C19—H19B	0.9800
Au3—Au20	3.1567 (15)	C19—H19C	0.9800
Au3—Au21	3.0971 (15)	C20—C46	1.50 (4)
Au3—S4	2.406 (6)	C21—H21A	0.9800
Au4—Au6	2.7630 (15)	C21—H21B	0.9800
Au4—Au7	2.7468 (16)	C21—H21C	0.9800
Au4—Au9	2.9127 (14)	C21—C61	1.48 (5)
Au4—Au12	3.1995 (15)	C22—H22A	0.9800
Au4—S2	2.356 (7)	C22—H22B	0.9800
Au5—Au8	2.8044 (15)	C22—H22C	0.9800
Au5—Au13	2.7308 (16)	C22—C40	1.48 (5)
Au5—Au17	2.9618 (15)	C23—H23A	0.9800
Au5—Au21	3.3659 (16)	C23—H23B	0.9800
Au5—S12	2.386 (7)	C23—H23C	0.9800
Au6—Au7	2.7208 (15)	C23—C24	1.59 (4)
Au6—Au10	2.9155 (15)	C24—C41	1.51 (5)
Au6—Au23	3.0665 (15)	C25—H25A	0.9800
Au6—S8	2.364 (6)	C25—H25B	0.9800
Au7—Au14	3.1545 (15)	C25—H25C	0.9800
Au7—Au15	3.2995 (16)	C25—C37	1.51 (5)
Au7—Au20	3.3657 (16)	C26—H26A	0.9800
Au7—S11	2.364 (7)	C26—H26B	0.9800
Au8—Au9	2.7606 (16)	C26—H26C	0.9800
Au8—Au13	2.7098 (16)	C26—C37	1.46 (6)
Au8—Au14	3.0384 (15)	C27—H27A	0.9800
Au8—Au16	2.8068 (16)	C27—H27B	0.9800
Au8—Au17	2.7976 (16)	C27—H27C	0.9800
Au8—Au22	2.8238 (15)	C28—H28A	0.9800
Au9—Au11	2.9225 (16)	C28—H28B	0.9800
Au9—Au12	2.7068 (15)	C28—H28C	0.9800
Au9—Au14	3.2801 (16)	C28—C53	1.51 (5)
Au9—Au16	2.7238 (15)	C29—C32	1.57 (5)
Au9—S1	2.370 (7)	C29—C58	1.45 (5)
Au10—Au13	2.9542 (15)	C30—H30A	0.9800
Au10—S3	2.323 (7)	C30—H30B	0.9800
Au10—S5	2.313 (7)	C30—H30C	0.9800
Au11—Au12	3.1782 (15)	C31—H31A	0.9800
Au11—Au19	3.2369 (15)	C31—H31B	0.9800

Au11—S2	2.296 (7)	C31—H31C	0.9800
Au11—S7	2.329 (7)	C31—C51	1.52 (4)
Au12—Au13	2.9076 (16)	C32—H32A	0.9800
Au12—Au16	2.6419 (15)	C32—H32B	0.9800
Au12—Au19	3.1648 (15)	C32—H32C	0.9800
Au12—Au24	3.2757 (16)	C34—H34A	0.9800
Au12—S3	2.358 (6)	C34—H34B	0.9800
Au13—Au16	3.2476 (15)	C34—H34C	0.9800
Au13—Au24	3.3269 (17)	C34—C51	1.52 (5)
Au13—S15	2.367 (7)	C33—H33A	0.9800
Au14—S1	2.306 (7)	C33—H33B	0.9800
Au14—S4	2.304 (7)	C33—H33C	0.9800
Au15—Au18	2.9192 (17)	C35—H35A	0.9800
Au15—Au20	3.0159 (16)	C35—H35B	0.9800
Au15—Au23	2.9543 (16)	C35—H35C	0.9800
Au15—S16	2.378 (7)	C36—H36A	0.9800
Au16—Au19	2.9179 (17)	C36—H36B	0.9800
Au16—Au22	3.2936 (17)	C36—H36C	0.9800
Au16—Au24	3.0477 (17)	C36—C51	1.52 (5)
Au16—S13	2.370 (7)	C37—C55	1.43 (6)
Au17—S4	2.321 (6)	C38—H38A	0.9800
Au17—S6	2.296 (7)	C38—H38B	0.9800
Au18—Au20	3.3688 (16)	C38—H38C	0.9800
Au18—Au21	3.1926 (16)	C39—C43	1.57 (6)
Au18—S10	2.307 (7)	C39—C48	1.55 (5)
Au18—S14	2.307 (7)	C39—C60	1.57 (6)
Au19—S7	2.314 (7)	C40—C44	1.45 (5)
Au19—S9	2.294 (7)	C40—C47	1.57 (5)
Au20—S10	2.318 (8)	C41—H41A	0.9800
Au20—S11	2.301 (8)	C41—H41B	0.9800
Au21—S12	2.316 (7)	C41—H41C	0.9800
Au21—S14	2.309 (7)	C42—H42A	0.9800
Au22—S6	2.302 (8)	C42—H42B	0.9800
Au22—S13	2.297 (8)	C42—H42C	0.9800
Au23—S8	2.289 (8)	C42—C57	1.43 (6)
Au23—S16	2.289 (8)	C43—H43A	0.9800
Au24—S9	2.310 (8)	C43—H43B	0.9800
Au24—S15	2.317 (8)	C43—H43C	0.9800
S1—C61	1.86 (3)	C44—H44A	0.9800
S2—C20	1.86 (3)	C44—H44B	0.9800
S3—C53	1.89 (3)	C44—H44C	0.9800
S4—C2	1.85 (3)	C45—H45A	0.9800
S5—C9	1.88 (3)	C45—H45B	0.9800
S6—C51	1.91 (3)	C45—H45C	0.9800
S7—C14	1.87 (4)	C45—C53	1.51 (4)
S8—C24	1.82 (3)	C46—H46A	0.9800
S9—C37	1.91 (5)	C46—H46B	0.9800
S10—C57	1.87 (4)	C46—H46C	0.9800

S11—C11	1.86 (3)	C47—H47A	0.9800
S12—C40	1.85 (3)	C47—H47B	0.9800
S13—C29	1.85 (4)	C47—H47C	0.9800
S14—C16	1.90 (3)	C48—H48A	0.9800
S15—C39	1.80 (4)	C48—H48B	0.9800
S16—C6	1.81 (3)	C48—H48C	0.9800
C1—H1A	0.9800	C49—H49A	0.9800
C1—H1B	0.9800	C49—H49B	0.9800
C1—H1C	0.9800	C49—H49C	0.9800
C1—C2	1.56 (4)	C49—C57	1.49 (6)
C2—C7	1.46 (4)	C50—H50A	0.9800
C2—C64	1.55 (3)	C50—H50B	0.9800
C3—H3A	0.9800	C50—H50C	0.9800
C3—H3B	0.9800	C52—H52A	0.9800
C3—H3C	0.9800	C52—H52B	0.9800
C3—C24	1.56 (5)	C52—H52C	0.9800
C4—H4A	0.9800	C54—H54A	0.9800
C4—H4B	0.9800	C54—H54B	0.9800
C4—H4C	0.9800	C54—H54C	0.9800
C4—C20	1.52 (4)	C55—H55A	0.9800
C5—H5A	0.9800	C55—H55B	0.9800
C5—H5B	0.9800	C55—H55C	0.9800
C5—H5C	0.9800	C56—H56A	0.9800
C5—C11	1.46 (6)	C56—H56B	0.9800
C6—C19	1.55 (5)	C56—H56C	0.9800
C6—C27	1.54 (5)	C58—H58A	0.9800
C6—C33	1.55 (4)	C58—H58B	0.9800
C7—H7A	0.9800	C58—H58C	0.9800
C7—H7B	0.9800	C59—H59A	0.9800
C7—H7C	0.9800	C59—H59B	0.9800
C8—H8A	0.9800	C59—H59C	0.9800
C8—H8B	0.9800	C59—C61	1.61 (5)
C8—H8C	0.9800	C60—H60A	0.9800
C8—C9	1.58 (4)	C60—H60B	0.9800
C9—C30	1.50 (5)	C60—H60C	0.9800
C9—C35	1.51 (5)	C61—C63	1.43 (6)
C10—H10A	0.9800	C62—H62A	0.9800
C10—H10B	0.9800	C62—H62B	0.9800
C10—H10C	0.9800	C62—H62C	0.9800
C10—C57	1.53 (5)	C63—H63A	0.9800
C11—C12	1.45 (5)	C63—H63B	0.9800
C11—C62	1.65 (6)	C63—H63C	0.9800
C12—H12A	0.9800	C64—H64A	0.9800
C12—H12B	0.9800	C64—H64B	0.9800
C12—H12C	0.9800	C64—H64C	0.9800

Au2—Au1—Au3	51.10 (3)	S11—Au20—Au18	139.68 (18)
Au2—Au1—Au9	176.23 (5)	S11—Au20—S10	175.1 (3)

Au2—Au1—Au10	67.10 (4)	Au2—Au21—Au5	53.21 (3)
Au2—Au1—Au12	132.27 (5)	Au2—Au21—Au18	88.69 (4)
Au2—Au1—Au14	114.60 (4)	Au3—Au21—Au2	51.34 (3)
Au4—Au1—Au2	123.02 (4)	Au3—Au21—Au5	57.92 (3)
Au4—Au1—Au3	117.71 (4)	Au3—Au21—Au18	61.08 (4)
Au4—Au1—Au5	174.73 (5)	Au18—Au21—Au5	119.01 (4)
Au4—Au1—Au9	59.00 (3)	S12—Au21—Au2	97.77 (18)
Au4—Au1—Au10	92.22 (4)	S12—Au21—Au3	89.49 (17)
Au4—Au1—Au12	64.69 (4)	S12—Au21—Au5	45.12 (18)
Au4—Au1—Au14	87.65 (4)	S12—Au21—Au18	135.82 (18)
Au5—Au1—Au2	61.00 (4)	S14—Au21—Au2	88.59 (18)
Au5—Au1—Au3	61.40 (4)	S14—Au21—Au3	96.35 (18)
Au5—Au1—Au9	116.77 (4)	S14—Au21—Au5	141.49 (18)
Au5—Au1—Au10	92.65 (4)	S14—Au21—Au18	46.21 (18)
Au5—Au1—Au12	115.74 (4)	S14—Au21—S12	173.2 (3)
Au5—Au1—Au14	87.42 (4)	Au8—Au22—Au16	53.96 (4)
Au6—Au1—Au2	64.11 (4)	S6—Au22—Au8	89.02 (17)
Au6—Au1—Au3	89.76 (4)	S6—Au22—Au16	142.68 (17)
Au6—Au1—Au4	59.98 (4)	S13—Au22—Au8	99.93 (17)
Au6—Au1—Au5	124.59 (5)	S13—Au22—Au16	46.02 (16)
Au6—Au1—Au9	118.44 (5)	S13—Au22—S6	170.6 (2)
Au6—Au1—Au10	58.82 (4)	Au15—Au23—Au6	73.10 (4)
Au6—Au1—Au12	95.38 (4)	S8—Au23—Au6	49.83 (16)
Au6—Au1—Au13	118.40 (5)	S8—Au23—Au15	121.81 (16)
Au6—Au1—Au14	122.66 (4)	S16—Au23—Au6	123.87 (17)
Au7—Au1—Au2	83.56 (4)	S16—Au23—Au15	52.07 (17)
Au7—Au1—Au3	57.58 (4)	S16—Au23—S8	173.7 (2)
Au7—Au1—Au4	60.15 (4)	Au12—Au24—Au13	52.25 (3)
Au7—Au1—Au5	118.84 (5)	Au16—Au24—Au12	49.23 (3)
Au7—Au1—Au6	60.02 (4)	Au16—Au24—Au13	61.07 (4)
Au7—Au1—Au8	122.84 (5)	S9—Au24—Au12	85.63 (19)
Au7—Au1—Au9	95.37 (4)	S9—Au24—Au13	137.77 (19)
Au7—Au1—Au10	118.70 (4)	S9—Au24—Au16	95.62 (19)
Au7—Au1—Au12	124.73 (5)	S9—Au24—S15	176.8 (3)
Au7—Au1—Au13	176.15 (6)	S15—Au24—Au12	97.45 (18)
Au7—Au1—Au14	62.90 (4)	S15—Au24—Au13	45.36 (18)
Au8—Au1—Au2	121.64 (5)	S15—Au24—Au16	85.8 (2)
Au8—Au1—Au3	97.10 (4)	Au14—S1—Au9	89.1 (2)
Au8—Au1—Au4	114.97 (5)	C61—S1—Au9	111.2 (12)
Au8—Au1—Au5	60.73 (4)	C61—S1—Au14	105.5 (12)
Au8—Au1—Au6	172.99 (6)	Au11—S2—Au4	94.1 (2)
Au8—Au1—Au9	56.04 (4)	C20—S2—Au4	111.5 (11)
Au8—Au1—Au10	118.38 (5)	C20—S2—Au11	104.8 (10)
Au8—Au1—Au12	77.75 (4)	Au10—S3—Au12	93.8 (2)
Au8—Au1—Au13	59.18 (4)	C53—S3—Au10	110.0 (11)
Au8—Au1—Au14	59.97 (4)	C53—S3—Au12	117.1 (9)
Au9—Au1—Au3	125.37 (4)	Au14—S4—Au3	94.3 (2)
Au9—Au1—Au10	116.46 (4)	Au14—S4—Au17	95.8 (2)

Au9—Au1—Au12	51.14 (3)	Au17—S4—Au3	120.0 (3)
Au9—Au1—Au14	61.81 (3)	C2—S4—Au3	118.6 (9)
Au10—Au1—Au3	118.17 (4)	C2—S4—Au14	115.1 (10)
Au10—Au1—Au12	65.51 (3)	C2—S4—Au17	109.6 (9)
Au10—Au1—Au14	178.00 (5)	Au10—S5—Au2	91.9 (2)
Au12—Au1—Au3	174.81 (4)	C9—S5—Au2	107.0 (10)
Au12—Au1—Au14	112.68 (4)	C9—S5—Au10	110.5 (11)
Au13—Au1—Au2	92.59 (4)	Au17—S6—Au22	100.9 (3)
Au13—Au1—Au3	119.63 (5)	C51—S6—Au17	107.1 (9)
Au13—Au1—Au4	122.64 (5)	C51—S6—Au22	102.9 (11)
Au13—Au1—Au5	58.66 (4)	Au19—S7—Au11	88.4 (2)
Au13—Au1—Au9	88.46 (4)	C14—S7—Au11	108.6 (12)
Au13—Au1—Au10	59.58 (4)	C14—S7—Au19	107.3 (12)
Au13—Au1—Au12	58.31 (4)	Au23—S8—Au6	82.4 (2)
Au13—Au1—Au14	118.91 (4)	C24—S8—Au6	107.7 (12)
Au14—Au1—Au3	63.58 (3)	C24—S8—Au23	104.7 (10)
Au1—Au2—Au6	55.05 (3)	Au19—S9—Au24	95.0 (3)
Au1—Au2—Au10	59.66 (3)	C37—S9—Au19	108.1 (13)
Au1—Au2—Au21	118.68 (4)	C37—S9—Au24	108.3 (12)
Au3—Au2—Au1	71.33 (4)	Au18—S10—Au20	93.5 (3)
Au3—Au2—Au5	67.91 (4)	C57—S10—Au18	106.5 (13)
Au3—Au2—Au6	96.67 (4)	C57—S10—Au20	106.6 (13)
Au3—Au2—Au10	130.95 (5)	Au20—S11—Au7	92.3 (2)
Au3—Au2—Au21	63.82 (4)	C11—S11—Au7	113.7 (14)
Au5—Au2—Au1	57.70 (3)	C11—S11—Au20	107.7 (11)
Au5—Au2—Au6	112.35 (4)	Au21—S12—Au5	91.4 (2)
Au5—Au2—Au10	86.72 (4)	C40—S12—Au5	109.7 (11)
Au5—Au2—Au21	67.66 (4)	C40—S12—Au21	106.6 (10)
Au6—Au2—Au10	54.11 (3)	Au22—S13—Au16	89.8 (2)
Au6—Au2—Au21	159.52 (5)	C29—S13—Au16	110.2 (13)
Au15—Au2—Au1	104.53 (5)	C29—S13—Au22	106.7 (13)
Au15—Au2—Au3	58.74 (4)	Au18—S14—Au21	87.5 (2)
Au15—Au2—Au5	126.58 (5)	C16—S14—Au18	107.8 (11)
Au15—Au2—Au6	77.85 (4)	C16—S14—Au21	108.0 (9)
Au15—Au2—Au10	130.46 (5)	Au24—S15—Au13	90.5 (3)
Au15—Au2—Au21	86.07 (4)	C39—S15—Au13	111.5 (13)
Au21—Au2—Au10	143.46 (5)	C39—S15—Au24	109.2 (13)
S5—Au2—Au1	94.89 (17)	Au23—S16—Au15	78.5 (2)
S5—Au2—Au3	152.45 (17)	C6—S16—Au15	114.6 (11)
S5—Au2—Au5	84.54 (17)	C6—S16—Au23	106.6 (11)
S5—Au2—Au6	94.24 (18)	H1A—C1—H1B	109.5
S5—Au2—Au10	43.44 (17)	H1A—C1—H1C	109.5
S5—Au2—Au15	148.71 (17)	H1B—C1—H1C	109.5
S5—Au2—Au21	106.02 (18)	C2—C1—H1A	109.5
Au2—Au3—Au1	57.58 (4)	C2—C1—H1B	109.5
Au2—Au3—Au5	59.37 (3)	C2—C1—H1C	109.5
Au2—Au3—Au7	83.57 (4)	C1—C2—S4	108 (2)
Au2—Au3—Au18	96.69 (4)	C7—C2—S4	109 (2)

Au2—Au3—Au20	120.68 (5)	C7—C2—C1	113 (2)
Au2—Au3—Au21	64.84 (4)	C7—C2—C64	112 (2)
Au5—Au3—Au1	51.99 (3)	C64—C2—S4	108.6 (19)
Au5—Au3—Au18	126.27 (4)	C64—C2—C1	106 (2)
Au5—Au3—Au20	169.49 (5)	H3A—C3—H3B	109.5
Au7—Au3—Au1	51.11 (3)	H3A—C3—H3C	109.5
Au7—Au3—Au5	103.01 (4)	H3B—C3—H3C	109.5
Au7—Au3—Au18	122.64 (4)	C24—C3—H3A	109.5
Au7—Au3—Au20	67.10 (4)	C24—C3—H3B	109.5
Au7—Au3—Au21	148.13 (5)	C24—C3—H3C	109.5
Au15—Au3—Au1	96.50 (4)	H4A—C4—H4B	109.5
Au15—Au3—Au2	60.39 (4)	H4A—C4—H4C	109.5
Au15—Au3—Au5	119.70 (5)	H4B—C4—H4C	109.5
Au15—Au3—Au7	72.59 (4)	C20—C4—H4A	109.5
Au15—Au3—Au18	59.12 (4)	C20—C4—H4B	109.5
Au15—Au3—Au20	61.97 (4)	C20—C4—H4C	109.5
Au15—Au3—Au21	87.39 (4)	H5A—C5—H5B	109.5
Au18—Au3—Au1	152.52 (4)	H5A—C5—H5C	109.5
Au20—Au3—Au1	118.21 (4)	H5B—C5—H5C	109.5
Au20—Au3—Au18	64.03 (4)	C11—C5—H5A	109.5
Au21—Au3—Au1	109.28 (4)	C11—C5—H5B	109.5
Au21—Au3—Au5	65.34 (4)	C11—C5—H5C	109.5
Au21—Au3—Au18	60.93 (4)	C19—C6—S16	106 (3)
Au21—Au3—Au20	124.90 (5)	C27—C6—S16	111 (3)
S4—Au3—Au1	88.56 (16)	C27—C6—C19	111 (3)
S4—Au3—Au2	133.61 (15)	C27—C6—C33	110 (3)
S4—Au3—Au5	75.07 (15)	C33—C6—S16	112 (2)
S4—Au3—Au7	99.60 (16)	C33—C6—C19	107 (3)
S4—Au3—Au15	164.17 (15)	C2—C7—H7A	109.5
S4—Au3—Au18	118.39 (16)	C2—C7—H7B	109.5
S4—Au3—Au20	102.44 (15)	C2—C7—H7C	109.5
S4—Au3—Au21	105.13 (16)	H7A—C7—H7B	109.5
Au1—Au4—Au9	65.99 (4)	H7A—C7—H7C	109.5
Au1—Au4—Au12	63.46 (4)	H7B—C7—H7C	109.5
Au6—Au4—Au1	59.30 (4)	H8A—C8—H8B	109.5
Au6—Au4—Au9	124.68 (5)	H8A—C8—H8C	109.5
Au6—Au4—Au12	94.25 (4)	H8B—C8—H8C	109.5
Au7—Au4—Au1	58.34 (4)	C9—C8—H8A	109.5
Au7—Au4—Au6	59.18 (4)	C9—C8—H8B	109.5
Au7—Au4—Au9	98.76 (5)	C9—C8—H8C	109.5
Au7—Au4—Au12	121.69 (5)	C8—C9—S5	105 (2)
Au9—Au4—Au12	52.32 (3)	C30—C9—S5	107 (2)
S2—Au4—Au1	150.25 (17)	C30—C9—C8	110 (3)
S2—Au4—Au6	128.39 (17)	C30—C9—C35	114 (3)
S2—Au4—Au7	151.21 (17)	C35—C9—S5	111 (2)
S2—Au4—Au9	96.04 (16)	C35—C9—C8	110 (3)
S2—Au4—Au12	86.80 (16)	H10A—C10—H10B	109.5
Au1—Au5—Au2	61.31 (4)	H10A—C10—H10C	109.5

Au1—Au5—Au3	66.60 (4)	H10B—C10—H10C	109.5
Au1—Au5—Au17	101.98 (4)	C57—C10—H10A	109.5
Au1—Au5—Au21	114.29 (4)	C57—C10—H10B	109.5
Au2—Au5—Au3	52.72 (3)	C57—C10—H10C	109.5
Au2—Au5—Au17	136.83 (5)	C5—C11—S11	113 (3)
Au2—Au5—Au21	59.13 (3)	C5—C11—C62	111 (4)
Au3—Au5—Au21	56.74 (3)	C12—C11—S11	107 (3)
Au8—Au5—Au1	58.11 (4)	C12—C11—C5	109 (4)
Au8—Au5—Au2	119.34 (5)	C12—C11—C62	112 (4)
Au8—Au5—Au3	98.86 (4)	C62—C11—S11	105 (3)
Au8—Au5—Au17	57.97 (4)	C11—C12—H12A	109.5
Au8—Au5—Au21	152.16 (5)	C11—C12—H12B	109.5
Au13—Au5—Au1	59.59 (4)	C11—C12—H12C	109.5
Au13—Au5—Au2	93.33 (4)	H12A—C12—H12B	109.5
Au13—Au5—Au3	125.71 (5)	H12A—C12—H12C	109.5
Au13—Au5—Au8	58.61 (4)	H12B—C12—H12C	109.5
Au13—Au5—Au17	112.61 (5)	H13A—C13—H13B	109.5
Au13—Au5—Au21	144.77 (5)	H13A—C13—H13C	109.5
Au17—Au5—Au3	84.24 (4)	H13B—C13—H13C	109.5
Au17—Au5—Au21	102.62 (4)	C20—C13—H13A	109.5
S12—Au5—Au1	153.80 (17)	C20—C13—H13B	109.5
S12—Au5—Au2	101.99 (17)	C20—C13—H13C	109.5
S12—Au5—Au3	87.26 (17)	C38—C14—S7	104 (3)
S12—Au5—Au8	132.26 (17)	C52—C14—S7	104 (2)
S12—Au5—Au13	145.78 (17)	C52—C14—C38	108 (3)
S12—Au5—Au17	75.91 (17)	C56—C14—S7	113 (2)
S12—Au5—Au21	43.46 (17)	C56—C14—C38	111 (3)
Au1—Au6—Au2	60.83 (4)	C56—C14—C52	116 (3)
Au1—Au6—Au4	60.72 (4)	H15A—C15—H15B	109.5
Au1—Au6—Au10	67.55 (4)	H15A—C15—H15C	109.5
Au1—Au6—Au23	139.89 (5)	H15B—C15—H15C	109.5
Au2—Au6—Au23	86.18 (4)	C16—C15—H15A	109.5
Au4—Au6—Au2	120.54 (5)	C16—C15—H15B	109.5
Au4—Au6—Au10	97.88 (4)	C16—C15—H15C	109.5
Au4—Au6—Au23	137.26 (5)	C15—C16—S14	103 (2)
Au7—Au6—Au1	59.11 (4)	C15—C16—C54	112 (3)
Au7—Au6—Au2	81.48 (4)	C50—C16—S14	111 (2)
Au7—Au6—Au4	60.11 (4)	C50—C16—C15	110 (3)
Au7—Au6—Au10	126.49 (5)	C50—C16—C54	116 (3)
Au7—Au6—Au23	96.28 (5)	C54—C16—S14	105 (2)
Au10—Au6—Au2	69.08 (4)	H17A—C17—H17B	109.5
Au10—Au6—Au23	123.85 (5)	H17A—C17—H17C	109.5
S8—Au6—Au1	167.43 (19)	H17B—C17—H17C	109.5
S8—Au6—Au2	116.94 (18)	C29—C17—H17A	109.5
S8—Au6—Au4	122.47 (18)	C29—C17—H17B	109.5
S8—Au6—Au7	133.45 (18)	C29—C17—H17C	109.5
S8—Au6—Au10	99.94 (18)	H18A—C18—H18B	109.5
S8—Au6—Au23	47.74 (18)	H18A—C18—H18C	109.5

Au1—Au7—Au3	71.31 (4)	H18B—C18—H18C	109.5
Au1—Au7—Au4	61.51 (4)	C53—C18—H18A	109.5
Au1—Au7—Au6	60.87 (4)	C53—C18—H18B	109.5
Au1—Au7—Au14	67.58 (4)	C53—C18—H18C	109.5
Au1—Au7—Au15	94.90 (4)	C6—C19—H19A	109.5
Au1—Au7—Au20	131.07 (5)	C6—C19—H19B	109.5
Au3—Au7—Au14	69.14 (4)	C6—C19—H19C	109.5
Au3—Au7—Au15	49.69 (3)	H19A—C19—H19B	109.5
Au3—Au7—Au20	59.77 (4)	H19A—C19—H19C	109.5
Au4—Au7—Au3	132.79 (5)	H19B—C19—H19C	109.5
Au4—Au7—Au14	90.77 (4)	C4—C20—S2	105 (2)
Au4—Au7—Au15	133.07 (5)	C13—C20—S2	112 (2)
Au4—Au7—Au20	167.33 (5)	C13—C20—C4	115 (3)
Au6—Au7—Au3	98.19 (5)	C13—C20—C46	110 (3)
Au6—Au7—Au4	60.70 (4)	C46—C20—S2	106 (2)
Au6—Au7—Au14	128.16 (5)	C46—C20—C4	108 (3)
Au6—Au7—Au15	72.41 (4)	H21A—C21—H21B	109.5
Au6—Au7—Au20	124.04 (5)	H21A—C21—H21C	109.5
Au14—Au7—Au15	118.55 (4)	H21B—C21—H21C	109.5
Au14—Au7—Au20	93.55 (4)	C61—C21—H21A	109.5
Au15—Au7—Au20	53.80 (3)	C61—C21—H21B	109.5
S11—Au7—Au1	173.06 (19)	C61—C21—H21C	109.5
S11—Au7—Au3	102.70 (19)	H22A—C22—H22B	109.5
S11—Au7—Au4	124.48 (19)	H22A—C22—H22C	109.5
S11—Au7—Au6	117.75 (18)	H22B—C22—H22C	109.5
S11—Au7—Au14	114.09 (18)	C40—C22—H22A	109.5
S11—Au7—Au15	78.36 (18)	C40—C22—H22B	109.5
S11—Au7—Au20	43.10 (19)	C40—C22—H22C	109.5
Au1—Au8—Au5	61.17 (4)	H23A—C23—H23B	109.5
Au1—Au8—Au9	68.85 (4)	H23A—C23—H23C	109.5
Au1—Au8—Au14	68.97 (4)	H23B—C23—H23C	109.5
Au1—Au8—Au16	101.51 (5)	C24—C23—H23A	109.5
Au1—Au8—Au17	108.68 (5)	C24—C23—H23B	109.5
Au1—Au8—Au22	160.54 (6)	C24—C23—H23C	109.5
Au5—Au8—Au14	92.47 (4)	C3—C24—S8	115 (2)
Au5—Au8—Au16	131.03 (5)	C3—C24—C23	105 (3)
Au5—Au8—Au22	109.00 (5)	C23—C24—S8	109 (2)
Au9—Au8—Au5	130.02 (5)	C41—C24—S8	108 (2)
Au9—Au8—Au14	68.70 (4)	C41—C24—C3	110 (3)
Au9—Au8—Au16	58.58 (4)	C41—C24—C23	108 (3)
Au9—Au8—Au17	138.31 (5)	H25A—C25—H25B	109.5
Au9—Au8—Au22	118.61 (5)	H25A—C25—H25C	109.5
Au13—Au8—Au1	60.92 (4)	H25B—C25—H25C	109.5
Au13—Au8—Au5	59.34 (4)	C37—C25—H25A	109.5
Au13—Au8—Au9	96.96 (5)	C37—C25—H25B	109.5
Au13—Au8—Au14	129.58 (5)	C37—C25—H25C	109.5
Au13—Au8—Au16	72.11 (4)	H26A—C26—H26B	109.5
Au13—Au8—Au17	118.68 (5)	H26A—C26—H26C	109.5

Au13—Au8—Au22	99.69 (5)	H26B—C26—H26C	109.5
Au16—Au8—Au14	125.61 (5)	C37—C26—H26A	109.5
Au16—Au8—Au22	71.60 (4)	C37—C26—H26B	109.5
Au17—Au8—Au5	63.84 (4)	C37—C26—H26C	109.5
Au17—Au8—Au14	71.85 (4)	C6—C27—H27A	109.5
Au17—Au8—Au16	149.39 (5)	C6—C27—H27B	109.5
Au17—Au8—Au22	78.17 (4)	C6—C27—H27C	109.5
Au22—Au8—Au14	130.07 (5)	H27A—C27—H27B	109.5
Au1—Au9—Au14	61.67 (3)	H27A—C27—H27C	109.5
Au4—Au9—Au1	55.00 (3)	H27B—C27—H27C	109.5
Au4—Au9—Au11	71.43 (4)	H28A—C28—H28B	109.5
Au4—Au9—Au14	85.45 (4)	H28A—C28—H28C	109.5
Au8—Au9—Au1	55.10 (3)	H28B—C28—H28C	109.5
Au8—Au9—Au4	110.03 (5)	C53—C28—H28A	109.5
Au8—Au9—Au11	152.17 (5)	C53—C28—H28B	109.5
Au8—Au9—Au14	59.66 (4)	C53—C28—H28C	109.5
Au11—Au9—Au1	118.22 (4)	C17—C29—S13	112 (3)
Au11—Au9—Au14	145.58 (5)	C17—C29—C32	108 (4)
Au12—Au9—Au1	65.62 (4)	C32—C29—S13	111 (2)
Au12—Au9—Au4	69.30 (4)	C58—C29—S13	104 (3)
Au12—Au9—Au8	85.63 (4)	C58—C29—C17	110 (3)
Au12—Au9—Au11	68.62 (4)	C58—C29—C32	113 (4)
Au12—Au9—Au14	126.91 (5)	C9—C30—H30A	109.5
Au12—Au9—Au16	58.22 (4)	C9—C30—H30B	109.5
Au16—Au9—Au1	94.53 (4)	C9—C30—H30C	109.5
Au16—Au9—Au4	127.01 (5)	H30A—C30—H30B	109.5
Au16—Au9—Au8	61.56 (4)	H30A—C30—H30C	109.5
Au16—Au9—Au11	94.67 (5)	H30B—C30—H30C	109.5
Au16—Au9—Au14	119.73 (5)	H31A—C31—H31B	109.5
S1—Au9—Au1	96.57 (17)	H31A—C31—H31C	109.5
S1—Au9—Au4	82.96 (16)	H31B—C31—H31C	109.5
S1—Au9—Au8	101.94 (17)	C51—C31—H31A	109.5
S1—Au9—Au11	105.77 (17)	C51—C31—H31B	109.5
S1—Au9—Au12	152.13 (17)	C51—C31—H31C	109.5
S1—Au9—Au14	44.65 (17)	C29—C32—H32A	109.5
S1—Au9—Au16	148.43 (17)	C29—C32—H32B	109.5
Au1—Au10—Au2	53.23 (3)	C29—C32—H32C	109.5
Au6—Au10—Au1	53.63 (3)	H32A—C32—H32B	109.5
Au6—Au10—Au2	56.81 (3)	H32A—C32—H32C	109.5
Au6—Au10—Au13	107.23 (4)	H32B—C32—H32C	109.5
Au13—Au10—Au1	53.60 (3)	H34A—C34—H34B	109.5
Au13—Au10—Au2	80.87 (4)	H34A—C34—H34C	109.5
S3—Au10—Au1	87.28 (16)	H34B—C34—H34C	109.5
S3—Au10—Au2	132.76 (17)	C51—C34—H34A	109.5
S3—Au10—Au6	79.92 (17)	C51—C34—H34B	109.5
S3—Au10—Au13	96.51 (16)	C51—C34—H34C	109.5
S5—Au10—Au1	90.16 (17)	C6—C33—H33A	109.5
S5—Au10—Au2	44.64 (16)	C6—C33—H33B	109.5

S5—Au10—Au6	97.92 (17)	C6—C33—H33C	109.5
S5—Au10—Au13	82.58 (17)	H33A—C33—H33B	109.5
S5—Au10—S3	177.3 (2)	H33A—C33—H33C	109.5
Au9—Au11—Au12	52.47 (3)	H33B—C33—H33C	109.5
Au9—Au11—Au19	85.19 (4)	C9—C35—H35A	109.5
Au12—Au11—Au19	59.11 (3)	C9—C35—H35B	109.5
S2—Au11—Au9	97.12 (18)	C9—C35—H35C	109.5
S2—Au11—Au12	88.32 (17)	H35A—C35—H35B	109.5
S2—Au11—Au19	136.74 (17)	H35A—C35—H35C	109.5
S2—Au11—S7	176.8 (2)	H35B—C35—H35C	109.5
S7—Au11—Au9	85.05 (19)	H36A—C36—H36B	109.5
S7—Au11—Au12	94.85 (18)	H36A—C36—H36C	109.5
S7—Au11—Au19	45.62 (17)	H36B—C36—H36C	109.5
Au1—Au12—Au4	51.85 (3)	C51—C36—H36A	109.5
Au1—Au12—Au11	109.23 (4)	C51—C36—H36B	109.5
Au1—Au12—Au24	118.49 (4)	C51—C36—H36C	109.5
Au4—Au12—Au24	170.00 (5)	C25—C37—S9	109 (4)
Au9—Au12—Au1	63.24 (4)	C26—C37—S9	110 (3)
Au9—Au12—Au4	58.38 (3)	C26—C37—C25	109 (3)
Au9—Au12—Au11	58.90 (4)	C55—C37—S9	104 (3)
Au9—Au12—Au13	93.63 (5)	C55—C37—C25	110 (4)
Au9—Au12—Au19	90.29 (4)	C55—C37—C26	115 (5)
Au9—Au12—Au24	121.97 (5)	C14—C38—H38A	109.5
Au11—Au12—Au4	64.56 (3)	C14—C38—H38B	109.5
Au11—Au12—Au24	124.95 (4)	C14—C38—H38C	109.5
Au13—Au12—Au1	53.80 (3)	H38A—C38—H38B	109.5
Au13—Au12—Au4	105.40 (4)	H38A—C38—H38C	109.5
Au13—Au12—Au11	152.36 (5)	H38B—C38—H38C	109.5
Au13—Au12—Au19	120.86 (5)	C43—C39—S15	109 (3)
Au13—Au12—Au24	64.78 (4)	C48—C39—S15	107 (3)
Au16—Au12—Au1	94.75 (4)	C48—C39—C43	108 (3)
Au16—Au12—Au4	119.16 (5)	C48—C39—C60	109 (3)
Au16—Au12—Au9	61.21 (4)	C60—C39—S15	113 (2)
Au16—Au12—Au11	90.60 (4)	C60—C39—C43	110 (4)
Au16—Au12—Au13	71.45 (4)	C22—C40—S12	113 (2)
Au16—Au12—Au19	59.52 (4)	C22—C40—C47	110 (3)
Au16—Au12—Au24	60.89 (4)	C44—C40—S12	108 (2)
Au19—Au12—Au1	150.71 (5)	C44—C40—C22	110 (3)
Au19—Au12—Au4	125.83 (4)	C44—C40—C47	110 (3)
Au19—Au12—Au11	61.37 (3)	C47—C40—S12	106 (2)
Au19—Au12—Au24	63.58 (4)	C24—C41—H41A	109.5
S3—Au12—Au1	86.29 (17)	C24—C41—H41B	109.5
S3—Au12—Au4	73.52 (17)	C24—C41—H41C	109.5
S3—Au12—Au9	131.85 (17)	H41A—C41—H41B	109.5
S3—Au12—Au11	103.91 (17)	H41A—C41—H41C	109.5
S3—Au12—Au13	96.96 (17)	H41B—C41—H41C	109.5
S3—Au12—Au16	164.28 (17)	H42A—C42—H42B	109.5
S3—Au12—Au19	122.38 (17)	H42A—C42—H42C	109.5

S3—Au12—Au24	104.91 (17)	H42B—C42—H42C	109.5
Au1—Au13—Au10	66.82 (4)	C57—C42—H42A	109.5
Au1—Au13—Au12	67.90 (4)	C57—C42—H42B	109.5
Au1—Au13—Au16	90.76 (4)	C57—C42—H42C	109.5
Au1—Au13—Au24	130.75 (5)	C39—C43—H43A	109.5
Au5—Au13—Au1	61.75 (4)	C39—C43—H43B	109.5
Au5—Au13—Au10	98.87 (5)	C39—C43—H43C	109.5
Au5—Au13—Au12	128.06 (5)	H43A—C43—H43B	109.5
Au5—Au13—Au16	117.07 (5)	H43A—C43—H43C	109.5
Au5—Au13—Au24	161.14 (5)	H43B—C43—H43C	109.5
Au8—Au13—Au1	59.90 (4)	C40—C44—H44A	109.5
Au8—Au13—Au5	62.05 (4)	C40—C44—H44B	109.5
Au8—Au13—Au10	126.27 (5)	C40—C44—H44C	109.5
Au8—Au13—Au12	82.75 (4)	H44A—C44—H44B	109.5
Au8—Au13—Au16	55.33 (4)	H44A—C44—H44C	109.5
Au8—Au13—Au24	109.40 (5)	H44B—C44—H44C	109.5
Au10—Au13—Au16	121.73 (5)	H45A—C45—H45B	109.5
Au10—Au13—Au24	99.47 (5)	H45A—C45—H45C	109.5
Au12—Au13—Au10	71.31 (4)	H45B—C45—H45C	109.5
Au12—Au13—Au16	50.46 (3)	C53—C45—H45A	109.5
Au12—Au13—Au24	62.97 (4)	C53—C45—H45B	109.5
Au16—Au13—Au24	55.22 (3)	C53—C45—H45C	109.5
S15—Au13—Au1	171.2 (2)	C20—C46—H46A	109.5
S15—Au13—Au5	121.1 (2)	C20—C46—H46B	109.5
S15—Au13—Au8	113.1 (2)	C20—C46—H46C	109.5
S15—Au13—Au10	119.1 (2)	H46A—C46—H46B	109.5
S15—Au13—Au12	106.9 (2)	H46A—C46—H46C	109.5
S15—Au13—Au16	80.53 (19)	H46B—C46—H46C	109.5
S15—Au13—Au24	44.1 (2)	C40—C47—H47A	109.5
Au1—Au14—Au9	56.52 (3)	C40—C47—H47B	109.5
Au7—Au14—Au1	49.53 (3)	C40—C47—H47C	109.5
Au7—Au14—Au9	83.78 (4)	H47A—C47—H47B	109.5
Au8—Au14—Au1	51.06 (3)	H47A—C47—H47C	109.5
Au8—Au14—Au7	100.57 (4)	H47B—C47—H47C	109.5
Au8—Au14—Au9	51.64 (3)	C39—C48—H48A	109.5
S1—Au14—Au1	93.38 (16)	C39—C48—H48B	109.5
S1—Au14—Au7	87.30 (16)	C39—C48—H48C	109.5
S1—Au14—Au8	95.73 (17)	H48A—C48—H48B	109.5
S1—Au14—Au9	46.26 (17)	H48A—C48—H48C	109.5
S4—Au14—Au1	90.45 (15)	H48B—C48—H48C	109.5
S4—Au14—Au7	95.62 (14)	H49A—C49—H49B	109.5
S4—Au14—Au8	86.23 (16)	H49A—C49—H49C	109.5
S4—Au14—Au9	136.50 (16)	H49B—C49—H49C	109.5
S4—Au14—S1	176.1 (2)	C57—C49—H49A	109.5
Au2—Au15—Au7	76.82 (4)	C57—C49—H49B	109.5
Au2—Au15—Au18	103.95 (5)	C57—C49—H49C	109.5
Au2—Au15—Au20	126.48 (5)	C16—C50—H50A	109.5
Au2—Au15—Au23	94.78 (5)	C16—C50—H50B	109.5

Au3—Au15—Au2	60.87 (4)	C16—C50—H50C	109.5
Au3—Au15—Au7	57.72 (4)	H50A—C50—H50B	109.5
Au3—Au15—Au18	70.05 (4)	H50A—C50—H50C	109.5
Au3—Au15—Au20	67.51 (4)	H50B—C50—H50C	109.5
Au3—Au15—Au23	139.70 (5)	C31—C51—S6	107 (2)
Au18—Au15—Au7	119.35 (5)	C34—C51—S6	113 (2)
Au18—Au15—Au20	69.15 (4)	C34—C51—C31	115 (3)
Au18—Au15—Au23	150.24 (5)	C34—C51—C36	109 (3)
Au20—Au15—Au7	64.22 (4)	C36—C51—S6	104 (2)
Au23—Au15—Au7	87.11 (4)	C36—C51—C31	108 (3)
Au23—Au15—Au20	117.14 (5)	C14—C52—H52A	109.5
S16—Au15—Au2	136.3 (2)	C14—C52—H52B	109.5
S16—Au15—Au3	162.6 (2)	C14—C52—H52C	109.5
S16—Au15—Au7	117.9 (2)	H52A—C52—H52B	109.5
S16—Au15—Au18	102.6 (2)	H52A—C52—H52C	109.5
S16—Au15—Au20	95.3 (2)	H52B—C52—H52C	109.5
S16—Au15—Au23	49.4 (2)	C18—C53—S3	102.9 (19)
Au8—Au16—Au13	52.56 (4)	C18—C53—C28	111 (3)
Au8—Au16—Au19	151.94 (5)	C18—C53—C45	112 (3)
Au8—Au16—Au22	54.44 (4)	C28—C53—S3	106 (2)
Au8—Au16—Au24	115.02 (5)	C45—C53—S3	111 (2)
Au9—Au16—Au8	59.86 (4)	C45—C53—C28	113 (3)
Au9—Au16—Au13	86.15 (4)	C16—C54—H54A	109.5
Au9—Au16—Au19	95.41 (5)	C16—C54—H54B	109.5
Au9—Au16—Au22	105.50 (5)	C16—C54—H54C	109.5
Au9—Au16—Au24	130.30 (5)	H54A—C54—H54B	109.5
Au12—Au16—Au8	85.94 (4)	H54A—C54—H54C	109.5
Au12—Au16—Au9	60.57 (4)	H54B—C54—H54C	109.5
Au12—Au16—Au13	58.08 (4)	C37—C55—H55A	109.5
Au12—Au16—Au19	69.19 (4)	C37—C55—H55B	109.5
Au12—Au16—Au22	135.87 (5)	C37—C55—H55C	109.5
Au12—Au16—Au24	69.88 (4)	H55A—C55—H55B	109.5
Au13—Au16—Au22	80.58 (4)	H55A—C55—H55C	109.5
Au19—Au16—Au13	117.84 (5)	H55B—C55—H55C	109.5
Au19—Au16—Au22	153.32 (5)	C14—C56—H56A	109.5
Au19—Au16—Au24	69.32 (4)	C14—C56—H56B	109.5
Au24—Au16—Au13	63.71 (4)	C14—C56—H56C	109.5
Au24—Au16—Au22	107.07 (5)	H56A—C56—H56B	109.5
S13—Au16—Au8	98.6 (2)	H56A—C56—H56C	109.5
S13—Au16—Au9	137.3 (2)	H56B—C56—H56C	109.5
S13—Au16—Au12	160.9 (2)	C10—C57—S10	104 (3)
S13—Au16—Au13	110.4 (2)	C42—C57—S10	107 (3)
S13—Au16—Au19	109.1 (2)	C42—C57—C10	111 (4)
S13—Au16—Au22	44.2 (2)	C42—C57—C49	111 (4)
S13—Au16—Au24	91.5 (2)	C49—C57—S10	111 (3)
Au8—Au17—Au5	58.19 (4)	C49—C57—C10	111 (4)
S4—Au17—Au5	79.90 (15)	C29—C58—H58A	109.5
S4—Au17—Au8	91.80 (17)	C29—C58—H58B	109.5

S6—Au17—Au5	105.3 (2)	C29—C58—H58C	109.5
S6—Au17—Au8	89.8 (2)	H58A—C58—H58B	109.5
S6—Au17—S4	174.5 (2)	H58A—C58—H58C	109.5
Au3—Au18—Au20	57.40 (3)	H58B—C58—H58C	109.5
Au15—Au18—Au3	50.83 (3)	H59A—C59—H59B	109.5
Au15—Au18—Au20	56.78 (4)	H59A—C59—H59C	109.5
Au15—Au18—Au21	81.01 (4)	H59B—C59—H59C	109.5
Au21—Au18—Au3	57.98 (3)	C61—C59—H59A	109.5
Au21—Au18—Au20	115.33 (5)	C61—C59—H59B	109.5
S10—Au18—Au3	86.50 (18)	C61—C59—H59C	109.5
S10—Au18—Au15	99.9 (2)	C39—C60—H60A	109.5
S10—Au18—Au20	43.37 (19)	C39—C60—H60B	109.5
S10—Au18—Au21	133.51 (19)	C39—C60—H60C	109.5
S10—Au18—S14	179.3 (3)	H60A—C60—H60B	109.5
S14—Au18—Au3	93.73 (17)	H60A—C60—H60C	109.5
S14—Au18—Au15	80.72 (18)	H60B—C60—H60C	109.5
S14—Au18—Au20	137.27 (18)	C21—C61—S1	107 (3)
S14—Au18—Au21	46.27 (17)	C21—C61—C59	109 (3)
Au12—Au19—Au11	59.52 (3)	C59—C61—S1	103 (2)
Au16—Au19—Au11	84.72 (4)	C63—C61—S1	113 (3)
Au16—Au19—Au12	51.29 (3)	C63—C61—C21	116 (4)
S7—Au19—Au11	46.00 (17)	C63—C61—C59	108 (4)
S7—Au19—Au12	95.52 (17)	C11—C62—H62A	109.5
S7—Au19—Au16	85.44 (19)	C11—C62—H62B	109.5
S9—Au19—Au11	135.2 (2)	C11—C62—H62C	109.5
S9—Au19—Au12	88.57 (19)	H62A—C62—H62B	109.5
S9—Au19—Au16	99.6 (2)	H62A—C62—H62C	109.5
S9—Au19—S7	174.8 (3)	H62B—C62—H62C	109.5
Au3—Au20—Au7	53.14 (3)	C61—C63—H63A	109.5
Au3—Au20—Au18	58.57 (3)	C61—C63—H63B	109.5
Au7—Au20—Au18	105.80 (4)	C61—C63—H63C	109.5
Au15—Au20—Au3	50.52 (3)	H63A—C63—H63B	109.5
Au15—Au20—Au7	61.98 (4)	H63A—C63—H63C	109.5
Au15—Au20—Au18	54.07 (4)	H63B—C63—H63C	109.5
S10—Au20—Au3	87.29 (18)	C2—C64—H64A	109.5
S10—Au20—Au7	140.32 (18)	C2—C64—H64B	109.5
S10—Au20—Au15	96.99 (18)	C2—C64—H64C	109.5
S10—Au20—Au18	43.12 (18)	H64A—C64—H64B	109.5
S11—Au20—Au3	97.56 (17)	H64A—C64—H64C	109.5
S11—Au20—Au7	44.57 (17)	H64B—C64—H64C	109.5
S11—Au20—Au15	85.61 (17)		

Au2—S5—C9—C8	−58 (2)	Au14—S1—C61—C63	41 (3)
Au2—S5—C9—C30	−174 (2)	Au14—S4—C2—C1	43 (2)
Au2—S5—C9—C35	61 (3)	Au14—S4—C2—C7	165.8 (16)
Au3—S4—C2—C1	−67 (2)	Au14—S4—C2—C64	−72 (2)
Au3—S4—C2—C7	55 (2)	Au15—S16—C6—C19	−157 (2)
Au3—S4—C2—C64	177.5 (16)	Au15—S16—C6—C27	83 (2)

Au4—S2—C20—C4	−74 (2)	Au15—S16—C6—C33	−40 (3)
Au4—S2—C20—C13	52 (3)	Au16—S13—C29—C17	161 (3)
Au4—S2—C20—C46	171.4 (17)	Au16—S13—C29—C32	41 (3)
Au5—S12—C40—C22	−53 (2)	Au16—S13—C29—C58	−81 (3)
Au5—S12—C40—C44	69 (3)	Au17—S4—C2—C1	149.5 (18)
Au5—S12—C40—C47	−173 (2)	Au17—S4—C2—C7	−87.7 (19)
Au6—S8—C24—C3	−46 (2)	Au17—S4—C2—C64	35 (2)
Au6—S8—C24—C23	−164 (2)	Au18—S10—C57—C10	−176 (2)
Au6—S8—C24—C41	78 (2)	Au18—S10—C57—C42	66 (3)
Au7—S11—C11—C5	−57 (3)	Au18—S10—C57—C49	−55 (3)
Au7—S11—C11—C12	−178 (3)	Au19—S7—C14—C38	163 (2)
Au7—S11—C11—C62	64 (3)	Au19—S7—C14—C52	−84 (3)
Au9—S1—C61—C21	176 (2)	Au19—S7—C14—C56	42 (3)
Au9—S1—C61—C59	62 (3)	Au20—S10—C57—C10	−77 (3)
Au9—S1—C61—C63	−55 (3)	Au20—S10—C57—C42	165 (3)
Au10—S3—C53—C18	81 (2)	Au20—S10—C57—C49	43 (3)
Au10—S3—C53—C28	−162.4 (18)	Au20—S11—C11—C5	44 (3)
Au10—S3—C53—C45	−39 (3)	Au20—S11—C11—C12	−77 (3)
Au10—S5—C9—C8	−156.3 (18)	Au20—S11—C11—C62	165 (3)
Au10—S5—C9—C30	87 (2)	Au21—S12—C40—C22	45 (2)
Au10—S5—C9—C35	−38 (3)	Au21—S12—C40—C44	167 (2)
Au11—S2—C20—C4	−174.7 (19)	Au21—S12—C40—C47	−75 (2)
Au11—S2—C20—C13	−49 (3)	Au22—S13—C29—C17	65 (3)
Au11—S2—C20—C46	71 (2)	Au22—S13—C29—C32	−55 (3)
Au11—S7—C14—C38	68 (3)	Au22—S13—C29—C58	−177 (3)
Au11—S7—C14—C52	−178 (2)	Au23—S8—C24—C3	41 (2)
Au11—S7—C14—C56	−52 (3)	Au23—S8—C24—C23	−77 (3)
Au12—S3—C53—C18	−173.6 (17)	Au23—S8—C24—C41	165 (2)
Au12—S3—C53—C28	−57 (2)	Au23—S16—C6—C19	−72 (3)
Au12—S3—C53—C45	66 (3)	Au23—S16—C6—C27	168 (2)
Au13—S15—C39—C43	−69 (3)	Au23—S16—C6—C33	44 (3)
Au13—S15—C39—C48	175 (2)	Au24—S15—C39—C43	−167 (3)
Au13—S15—C39—C60	55 (3)	Au24—S15—C39—C48	76 (3)
Au14—S1—C61—C21	−89 (3)	Au24—S15—C39—C60	−44 (3)
Au14—S1—C61—C59	157 (2)		