Electronic Supplementary Information (ESI)

Hierarchical Multi-shell 66-Nuclei Silver Nanoclusters Trapping Subvalent Ag_6 Kernels

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Experimental details

The precursors, $(^{i}PrSAg)_n$ and $(^{i}BuSAg)_n$[1] and the POMs template of $(^{n}Bu_4N)_4(Mo_8O_{26})$[2] were prepared by following the reported procedures. All chemicals and solvents used in the syntheses were of analytical grade and used without further purification. ^{i}PrSH (Adamas-beta®) and ^{i}BuSH (Adamas-beta®) were purchased from Shanghai Titan Scientific Co.,Ltd. The elemental analyses (C, H contents) were determined on a Vario EL III analyzer. The diffuse-reflectance spectrum were performed on UV−Vis spectrophotometer (Evolution 220, ISA-220 accessory, Thermo Scientific) using a built-in 10 mm silicon photodiode with a 60 mm Spectralon sphere. Morphology of the samples and elemental composition analyses were measured using an SU-8010 field emission scanning electron microscope (FESEM; Hitachi Ltd., Tokyo, Japan) equipped with an Oxford-Horiba Inca XMax50 energy dispersive X-ray spectroscopy (EDS) attachment (Oxford Instruments Analytical, High Wycombe, England). Mass spectra were recorded on an Agilent 6224 (Agilent Technologies, USA) ESI-TOF-MS spectrometer. Sample solutions are infused by a syringe pump at 4 μL/min. Data were acquired using the following settings: ESI capillary voltage was set at 3500 V (−) ion mode and fragmentor at 200 V. The liquid nebulizer was set to 15 psig and the nitrogen drying gas was set to a flow rate of 4 L/min. Drying gas temperature was maintained at 150 ^{o}C. The data analyses of mass spectra were performed based on the isotope distribution patterns using Agilent MassHunter Workstation Data acquisition software (Version B.05.00). The reported *m/z* values represent monoisotopic mass of the most abundant peak within the isotope pattern. ^{13}C NMR spectrum was recorded in a J. Young NMR tube on Bruker Avance 500 spectrometers. The chemical shifts are reported in parts per million δ (ppm) referenced to the residual proton signal of the deuterated methanol. X-ray photoelectron spectra (XPS) were recorded with a Quantum 2000 X-ray scanning ESCA microprobe. The single crystals were put under UHV to reach the 10^{-8} Pa range. The nonmonochromatized Al *K*α source was used at 10 kV and 10 mA. The binding energy of the spectrum was calibrated in relation to the C 1s binging energy (284.0 eV), which was applied as an internal standard.

X-ray crystallography

Data Collection and Treatment Details

Single crystal of **SD/Ag66b-SD/Ag66d** with appropriate dimensions was chosen under an optical microscope and quickly coated with high vacuum grease (Dow Corning Corporation) to prevent decomposition. Single-crystal X-ray diffraction data of **SD/Ag66b** was collected on a Rigaku Oxford Diffraction XtaLAB Synergy diffractometer equipped with a HyPix-6000HE area detector at 100 K using Mo Kα (λ = 0.71073 Å) from PhotonJet micro-focus X-ray Source. The diffraction images were processed and scaled using the CrysAlisPro software.[3] Single-crystal X-ray diffraction data of **SD/Ag66c** and **SD/Ag66d** were recorded on a Bruker Apex II single crystal diffractometer and a CCD area detector at 173 and 100 K. The raw frame data were processed using SAINT and SADABS to yield the reflection data file.[4] The structure was solved using the charge-flipping algorithm, as implemented in the program *SUPERFLIP*[5] and refined by full-matrix least-squares techniques against F_o^2 using the SHELXL program[6] through the OLEX2 interface.[7] Hydrogen atoms at carbon were placed in calculated positions and refined isotropically by using a riding model. Appropriate restraints or constraints were applied to the geometry and the atomic displacement parameters of the atoms in the cluster. All structures were examined using the Addsym subroutine of PLATON[8] to ensure that no additional symmetry could be applied to the models. Pertinent crystallographic data collection and refinement parameters are collated in Table S2. Selected bond lengths and angles are collated in Table S3.

Specific Refinement Details

The crystals of **SD/Ag66b-SD/Ag66d** were weakly diffracting with very few reflections recorded at higher than 0.9 Å resolution. Due to the wide presence of disordered groups in three clusters, structural refinements are very challenging and several restraint commands were widely used during the refinements.

For **SD/Ag66b**, all non-H atoms were located in the electron density and refined with anisotropic thermal parameters. Due to the less than ideal resolution, DFIX restraints were applied to keep the bond lengths (C=O bond 1.25 Å and C-C bond 1.55 Å) in reasonable ranges. FLAT restraints were applied to keep the planarity of carboxylate group with one attached C atom or benzene ring. SIMU

restraints were also used for some ligands with large thermal motion as well as two disordered silver atoms. The more detailed information can be found in '_olex2_refinement_description' loop in CIF file.

For **SD/Ag66c**, all non-H atoms were located in the electron density and all Ag, Mo, S atoms were refined with anisotropic thermal parameters. Partial light atoms (C and O) were refined with isotropic thermal parameters due to the large thermal motion or some unresolved disorder which could not be modeled despite many attempts. Due to the less than ideal resolution, DFIX restraints were applied to keep the bond lengths (C=O bond 1.25 Å; C-S bond 1.85 Å and C-C bond 1.55 Å) in reasonable ranges. FLAT restraints were applied to keep the planarity of carboxylate group with one attached C atom or benzene ring. SIMU restraints were also used for some ligands with large thermal motion as well as some disordered silver atoms. AFIX 66 was used for some benzene rings to keep their normal geometry like hexagon. The more detailed information can be found in '_olex2_refinement_description' loop in CIF file.

For **SD/Ag66d**, all non-H atoms were located in the electron density and all Ag, Mo, S atoms were refined with anisotropic thermal parameters. Partial light atoms (C and O) were refined with isotropic thermal parameters due to the large thermal motion or some unresolved disorder which could not be modeled despite many attempts. Due to the less than ideal resolution, DFIX restraints were applied to keep the bond lengths (C=O bond 1.25 Å; C-S bond 1.85 Å and C-C bond 1.55 Å) in reasonable ranges. FLAT restraints were applied to keep the planarity of carboxylate group with one attached C atom or benzene ring. SIMU restraints were also used for some ligands with large thermal motion as well as some disordered silver atoms. The more detailed information can be found in '_olex2_refinement_description' loop in CIF file.

For **SD/Ag66c** and **SD/Ag66d**, the lattices contain large solvents and anions accessible voids, but they are highly disordered and therefore could not be modelled. Instead, they are treated by the program SQUEEZE.[9] These electrons removed by SQUEEZE have been assigned as some solvents and anions. The more detailed information can be found in '_platon_squeeze_details' loop in CIF file.

In all, despite an R_1 value that was not very good and resolution that was poorer than generally obtained in crystallography of some small molecules, a reasonable quality refinement was achieved, and the current data is more than adequate for establishing the average connectivity of the structure.

Synthesis Details

Synthesis of SD/Ag66b

PhCOOAg (0.1 mmol, 27.9 mg) and (^{i}PrSAg)$_n$ (0.05 mmol, 9.2 mg) together with [(n-C_4H_9)$_4$N]$_4$[α-Mo_8O_{26}] (0.0002 mmol, 4.2 mg) were dissolved in a mixed solvent of methanol : *N,N'*-dimethylformamide (5 mL v/v = 1/1). The reaction mixture was sealed and heated at 65 ^{o}C for 2000 min, and then cooled to room temperature for 800 min. Then the yellow crystals of **SD/Ag66b** were crystallized in the yields of 11 %.

Synthesis of SD/Ag66c

The synthetic condition was similar to that described for **SD/Ag66b**, except that the (^{i}PrSAg)$_n$ was substituted by (^{i}BuSAg)$_n$ (0.05 mmol, 9.9 mg), then the yellow crystals of **SD/Ag66c** were crystallized in the yields of 12 %.

Synthesis of SD/Ag66d

The synthetic condition was similar to that described for **SD/Ag66b**, except that the PhCOOAg was substituted by AgOAc (0.1 mmol, 16.7 mg). After cooling to room temperature, the colorless solution was filtered and the filtrate left to evaporate slowly for one month in the dark at room temperature. Pale yellow crystals of **SD/Ag66d** were crystallized in a yield of 15 %.

Figure S1: a) Crystal structure of **SD/Ag66c**; b) side view of crystal structure of **SD/Ag66c**; c) core structure of **SD/Ag66c**. Hydrogen atoms are omitted for clarity. Color legend: Pink/dark blue Ag; gray C; red O; yellow S. The MoO_4 units are represented as the green tetrahedron; the innermost Ag_6 is differentiated as dark blue.

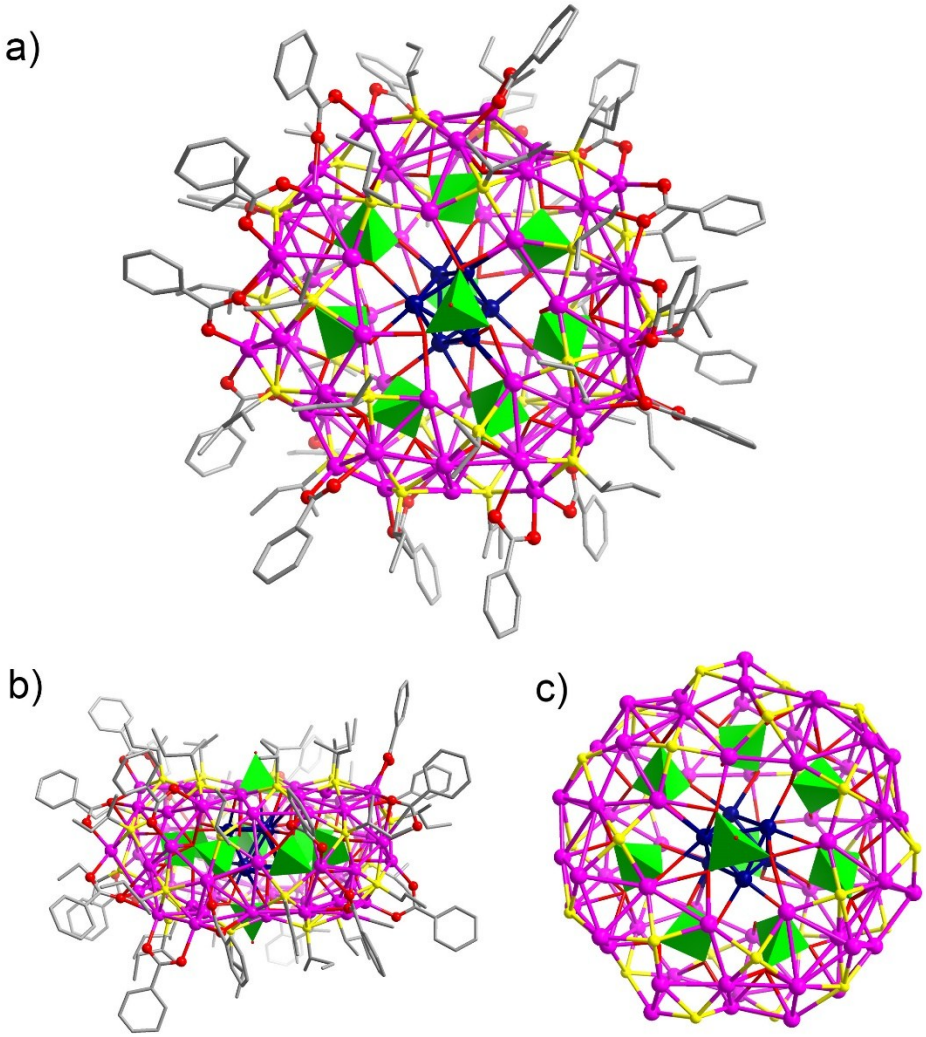


Figure S2: a) Crystal structure of **SD/Ag66d**; b) side view of crystal structure of **SD/Ag66d**; c) core structure of **SD/Ag66d**. Hydrogen atoms are omitted for clarity. Color legend: Pink/dark blue Ag; gray C; red O; yellow S. The MoO_4 units are represented as the green tetrahedron; the innermost Ag_6 is differentiated as dark blue.

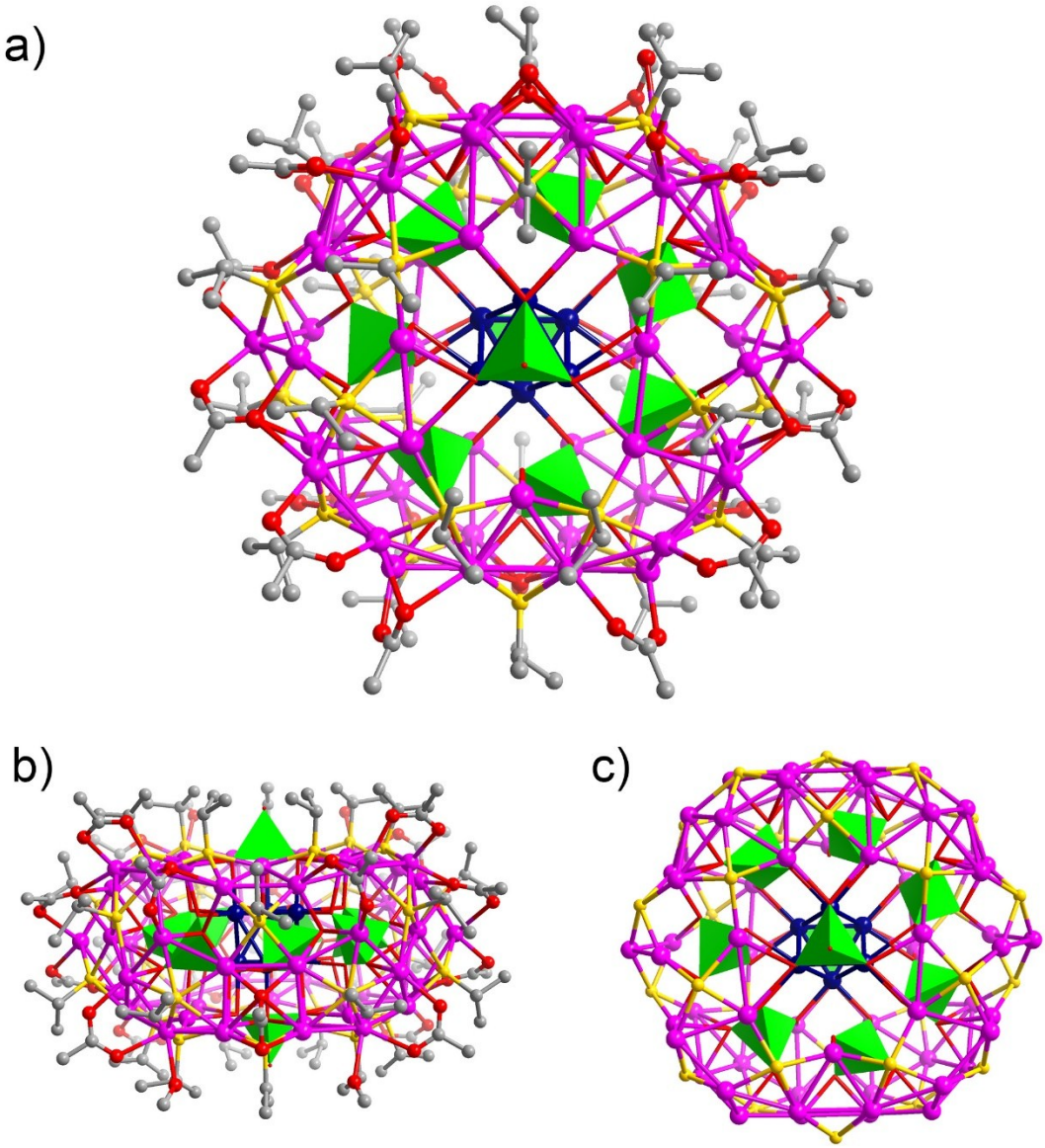


Figure S3: Core size of **SD/Ag66b**

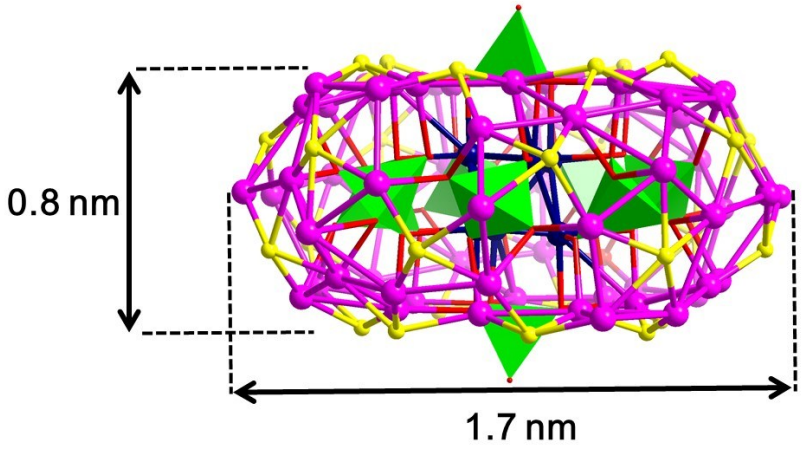


Figure S4: Coordination modes of benzoate ions in the Ag_{60} shell. The μ_4-*O,O',O',O'* bridged benzoate ions filling the gaps between the pentagons and tetragons are shown in green. The pentagons are highlighted as bold brown.

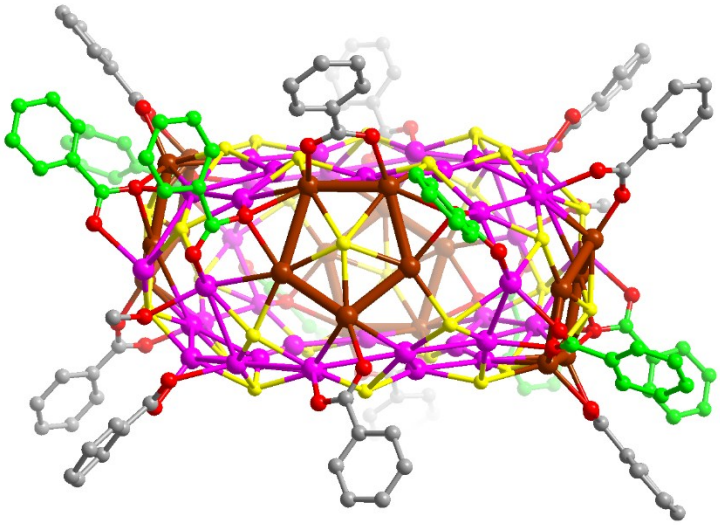


Figure S5: High resolution XPS spectrum of Ag $3d_{5/2}$.

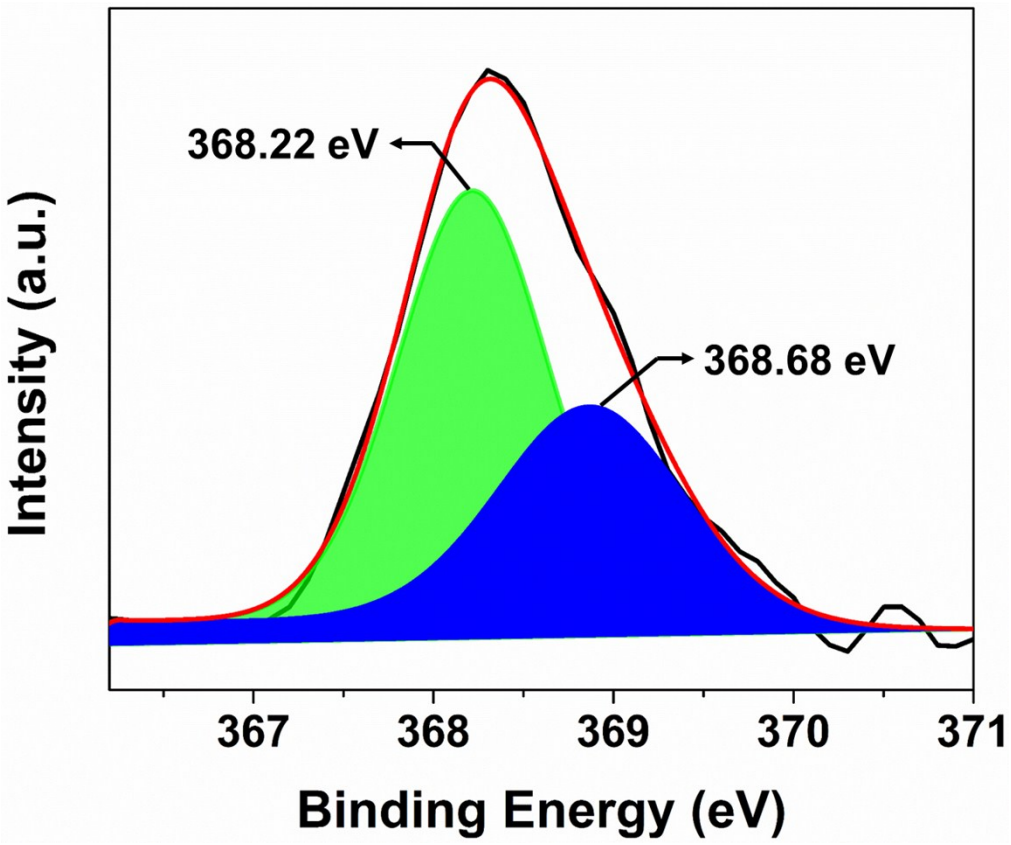


Figure S6: ^{13}C NMR of HCl digested reaction mother solution for **SD/Ag66d**.

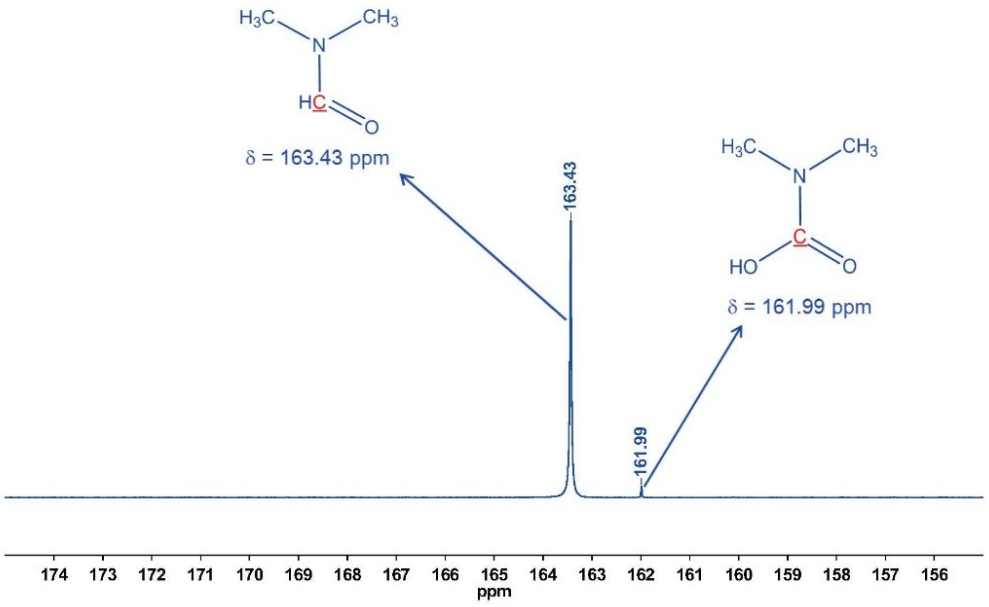


Figure S7: a) Asymmetric unit of **SD**/**Ag66b** with seven positions of Mo are identified with half occupation at the equatorial region. b) whole cluster of **SD**/**Ag66b** with the half occupied 14 positions of Mo linking into a circle. Color legend: Pink Ag; gray C; aquamarine Mo; red O; yellow S; pale white H.

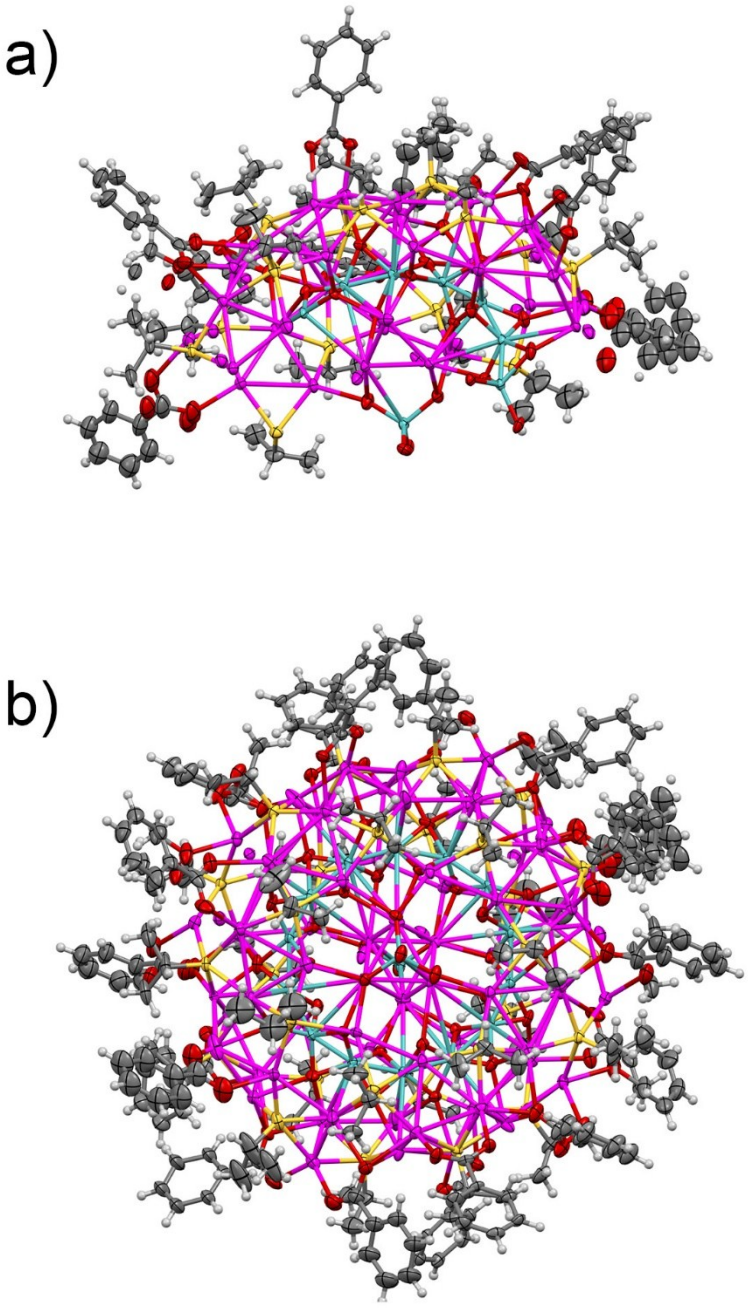


Figure S8: The theoretical and experimental isotope distributions of species **3a-3h.**

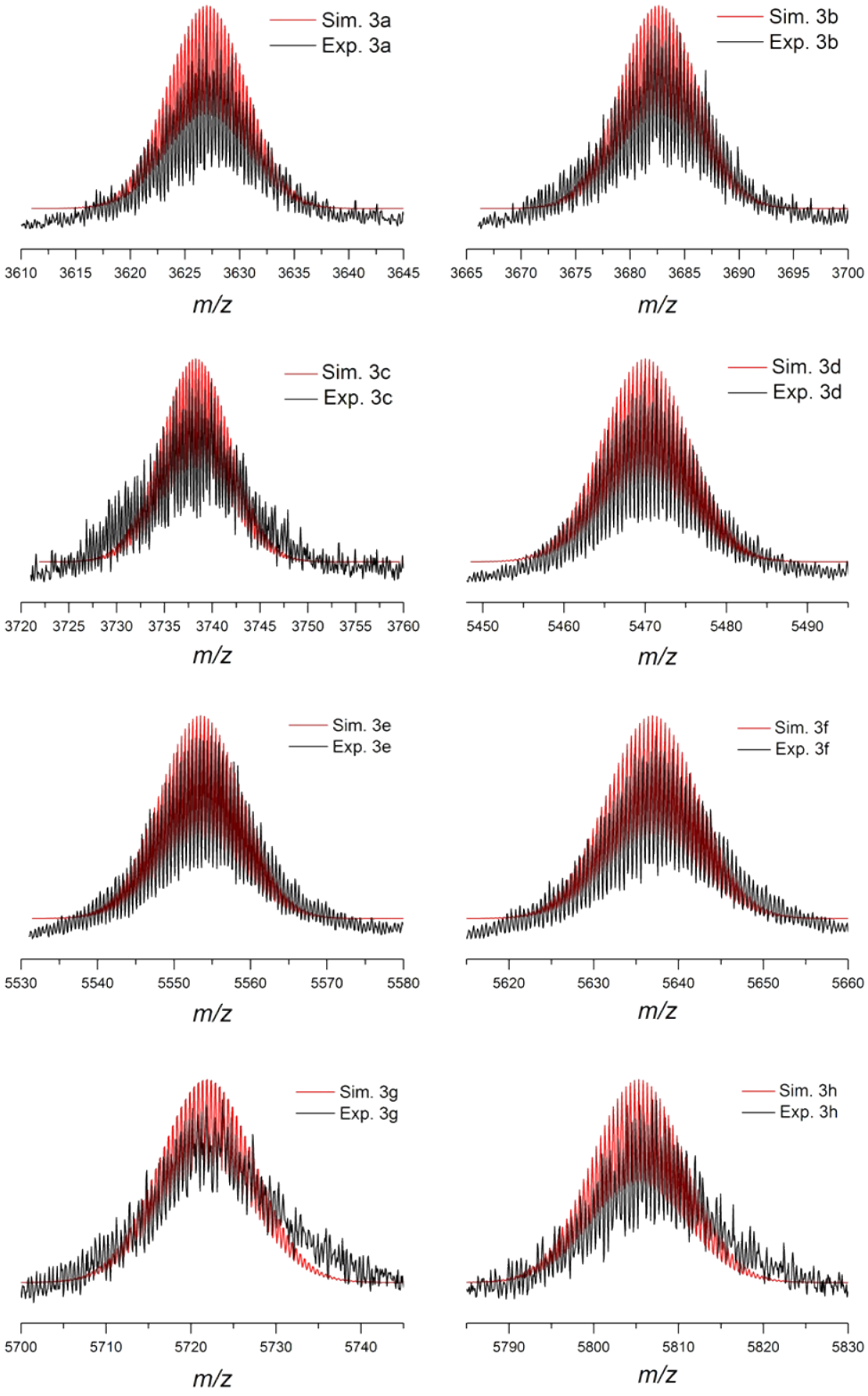


Figure S9: Energy gap (E_g) obtained from UV-Vis spectrum.

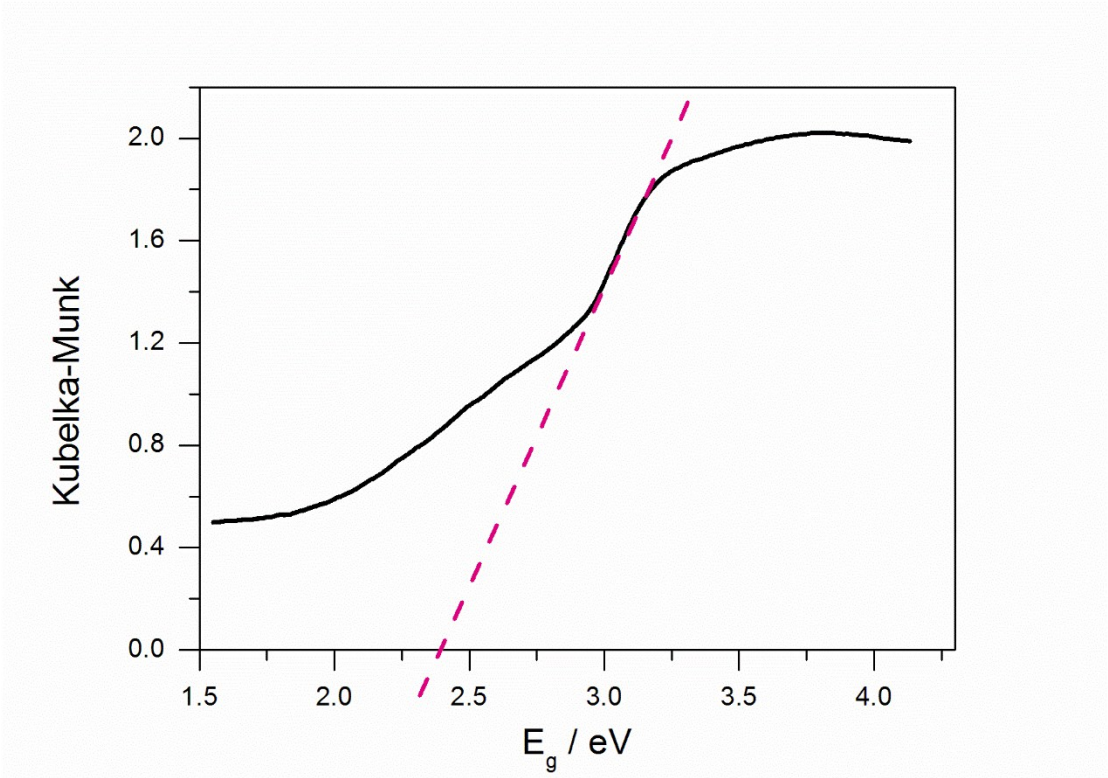


Figure S10. The plot of maximum of the intensities (I_{max}) against temperature shows a good linear relationship

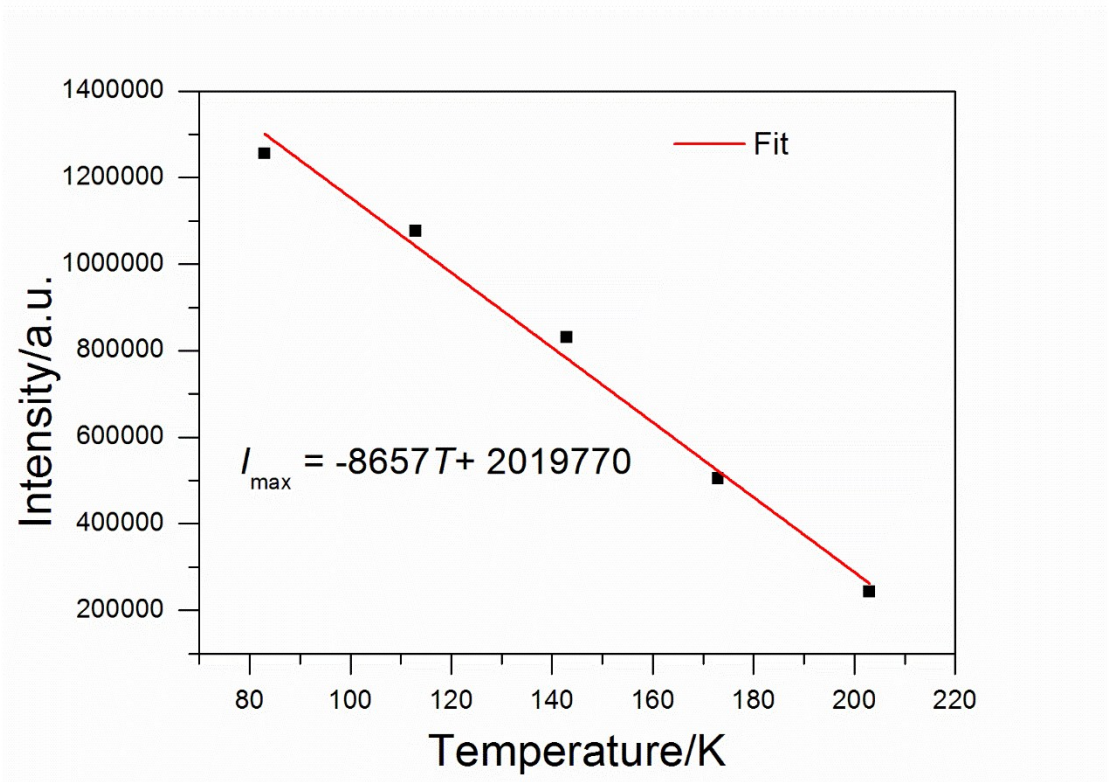


Figure S11. The emission at 83 K shows single-exponential behavior with life time τ = 153 μs.

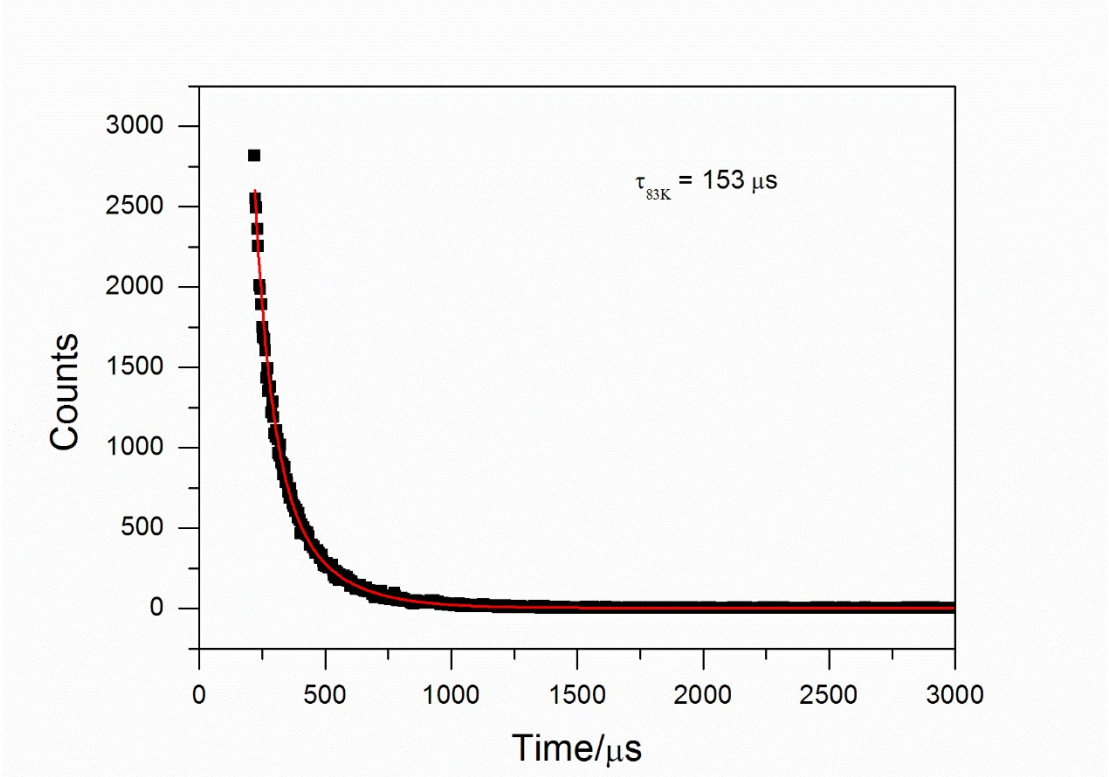


Figure S12: Comparison of observed and simulated PXRD patterns of **SD/Ag66d**.

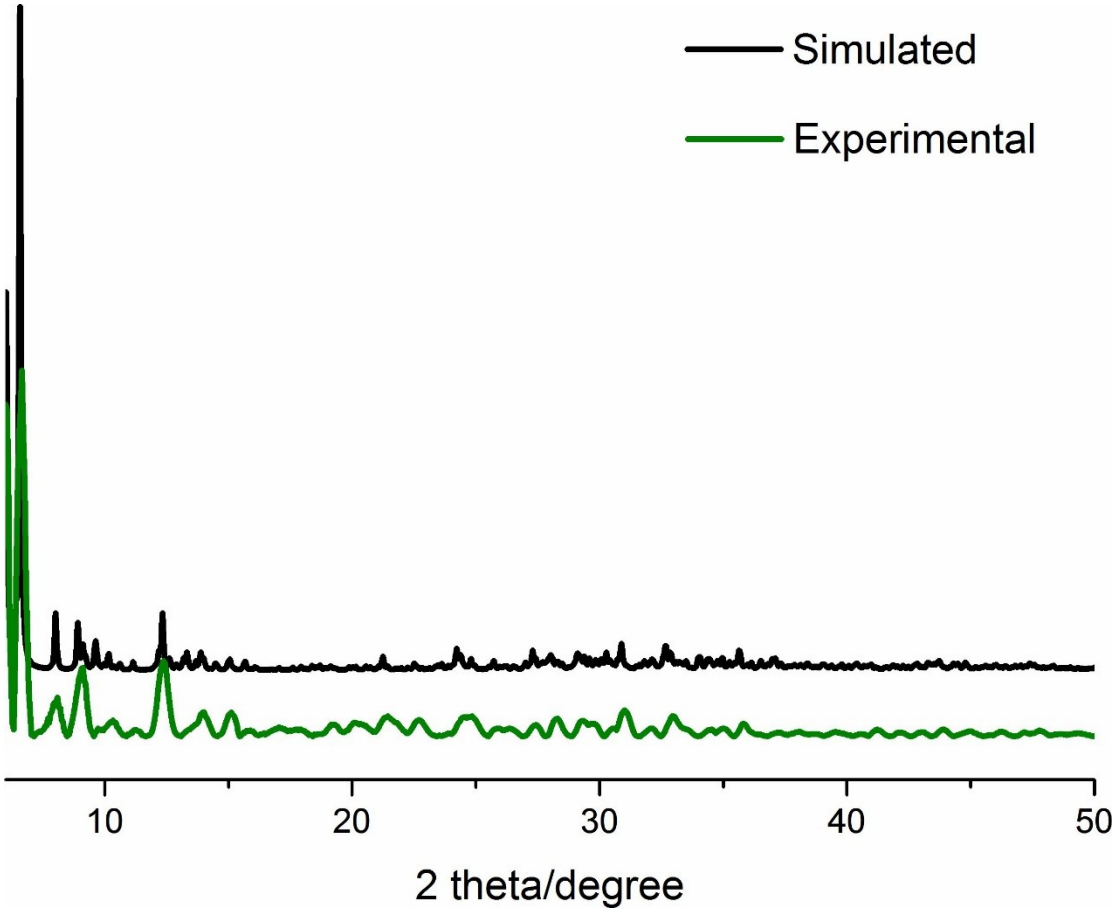


Figure S13: SEM and elemental mapping images of **SD/Ag66d**.

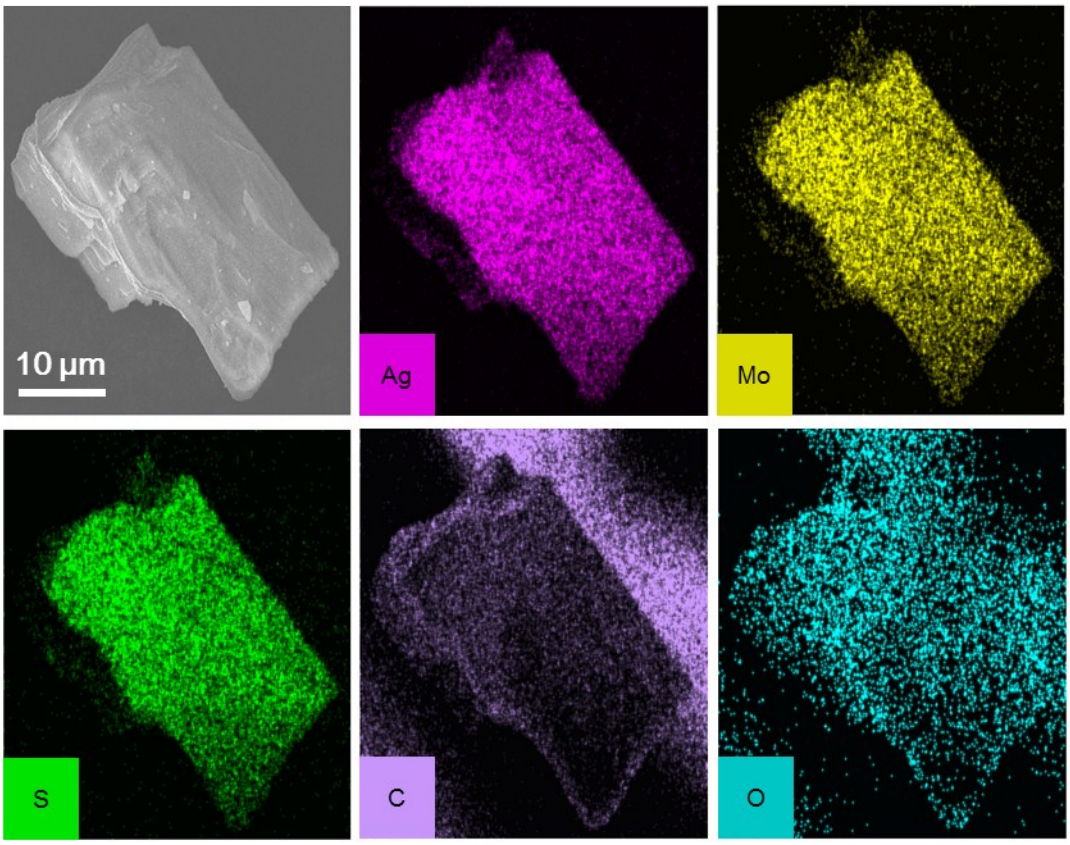
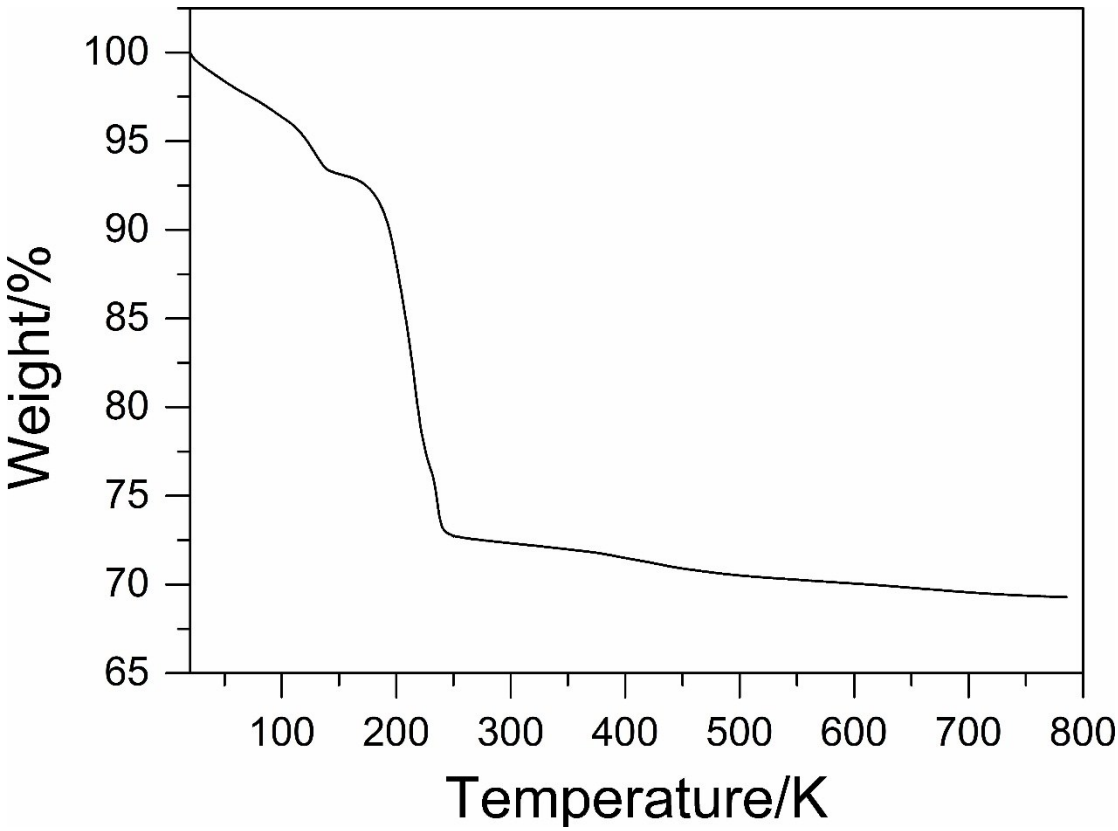


Figure S14: TGA curve of **SD/Ag66d**.



As shown in Fig. S14, we tested the thermal stability using TGA for **SD/Ag66d**. The result showed the **SD/Ag66d** quickly loses solvents even starting from room temperature. When heating to 135 ^{o}C, almost all solvents are removed. The main skeleton of cluster starts to decompose at 178 ^{o}C.

Table S1: The assigned formula of species found in ESI-MS of **SD/Ag66d** dissolved in CH_2Cl_2.

Peaks for SD/Ag66d	**Species**	**Exp. *m/z***	**Sim. *m/z***
3a	$[Ag_6@(MoO_4)_9@Ag_{56}(^{i}PrS)_{28}(OAc)_{11}]^{3+}$	3626.95	3626.99
3b	$[Ag_6@(MoO_4)_9@Ag_{57}(^{i}PrS)_{28}(OAc)_{12}]^{3+}$	3682.58	3682.63
3c	$[Ag_6@(MoO_4)_9@Ag_{58}(^{i}PrS)_{28}(OAc)_{13}]^{3+}$	3738.24	3738.27
3d	$[Ag_6@(MoO_4)_9@Ag_{56}(^{i}PrS)_{28}(OAc)_{12}]^{2+}$	5469.88	5469.99
3e	$[Ag_6@(MoO_4)_9@Ag_{57}(^{i}PrS)_{28}(OAc)_{13}]^{2+}$	5553.34	5553.45
3f	$[Ag_6@(MoO_4)_9@Ag_{58}(^{i}PrS)_{28}(OAc)_{14}]^{2+}$	5636.80	5636.91
3g	$[Ag_6@(MoO_4)_9@Ag_{58}(^{i}PrS)_{28}(OAc)_{14}(CH_2Cl_2)_2]^{2+}$	5721.80	5721.86
3h	$[Ag_6@(MoO_4)_9@Ag_{59}(^{i}PrS)_{28}(OAc)_{15}(CH_2Cl_2)_2]^{2+}$	5805.46	5805.32

Table S2: Crystal data collection and structure refinement for **SD/Ag66b-SD/Ag66d**.

Compound	**SD/Ag66b**	**SD/Ag66c**	**SD/Ag66d**
Empirical formula	$C_{212}H_{292}Ag_{66}Mo_9O_{74}S_{28}$	$C_{234.5}H_{339.5}Ag_{66}Mo_9O_{71}S_{28}$	$C_{120}H_{260}Ag_{66}Mo_9O_{72}S_{28}$
X-ray diffractometer	Rigaku Oxford Diffraction XtaLAB Synergy	Bruker APEX II	Bruker APEX II
Formula weight	12905.00	13175.10	11735.82
Temperature/K	100.00(13)	173(2)	100(2)
Crystal system	triclinic	monoclinic	orthorhombic
Space group	P-1	$P2_1/c$	Pnnm
a/Å	16.3935(2)	17.8507(15)	19.780(2)
b/Å	23.8317(3)	46.314(4)	21.915(3)
c/Å	24.0155(3)	44.484(4)	33.362(4)
α/°	112.6803(13)	90	90
β/°	108.2811(12)	99.760(2)	90
γ/°	99.7127(12)	90	90
Volume/Å^3	7757.8(2)	36244(5)	14462(3)
Z	1	4	2
ρ_{calc}g/cm^3	2.762	2.415	2.695
μ/mm^{-1}	4.654	3.987	4.978
F(000)	6084.0	24970.0	10968.0
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
Reflections collected	102945	216447	99413
Independent reflections	31603 [R_{int} = 0.0472, R_{sigma} = 0.0484]	63713 [R_{int} = 0.0496, R_{sigma} = 0.0585]	12945 [R_{int} = 0.0518, R_{sigma} = 0.0300]
Data/parameters	31603/2013	63713/3351	12945/759
Goodness-of-fit on F^2	1.092	1.030	1.865
Final R indexes [I>=2σ (I)]	R_1 = 0.0601, wR_2 = 0.1211	R_1 = 0.0836, wR_2 = 0.1957	R_1 = 0.1224, wR_2 = 0.3601
Final R indexes [all data]	R_1 = 0.0780, wR_2 = 0.1286	R_1 = 0.1338, wR_2 = 0.2306	R_1 = 0.1544, wR_2 = 0.4344
Largest diff. peak/hole / e Å^{-3}	2.95/-3.48	3.62/-2.01	7.02/-4.61

Table 3: Selected bond distances (Å) and angles (˚) for **SD/Ag66b-SD/Ag66d**.

SD/Ag66b			
Ag1—Ag2	2.693 (3)	Ag16—S11	2.558 (4)
Ag1—Ag2^{i}	2.855 (3)	Ag16—S12	2.585 (3)
Ag1—Ag10	2.708 (3)	Ag16—O24	2.402 (9)
Ag1—Ag10^{i}	2.798 (3)	Ag16—O25	2.321 (10)
Ag1—Ag31	3.330 (2)	Ag17—S13	2.533 (3)
Ag1—O2^{i}	2.316 (7)	Ag17—O5	2.508 (7)
Ag1—O10	2.376 (8)	Ag17—O19	1.950 (7)
Ag2—Ag1^{i}	2.855 (3)	Ag18—S8	2.534 (3)
Ag2—Ag10	2.8306 (13)	Ag18—S11	2.463 (3)
Ag2—Ag10^{i}	2.6998 (13)	Ag18—O13	2.464 (8)
Ag2—O4	2.377 (7)	Ag18—O26	2.477 (8)
Ag2—O7	2.352 (7)	Ag19—Ag20	2.8112 (13)
Ag2—O9	2.587 (7)	Ag19—Ag23	2.9102 (13)
Ag3—Ag5^{i}	3.332 (6)	Ag19—S9	2.518 (3)
Ag3—Ag6^{i}	3.159 (4)	Ag19—S12	2.484 (3)
Ag3—Ag11	3.019 (2)	Ag19—O13	2.393 (8)
Ag3—Ag17	2.659 (4)	Ag19—O26	2.527 (8)
Ag3—S1^{i}	2.587 (3)	Ag20—Ag21	2.8153 (13)
Ag3—S13	2.468 (4)	Ag20—Ag24	3.1530 (12)
Ag3—O3	2.224 (9)	Ag20—Ag25	2.9551 (12)
Ag4—Ag12	2.974 (3)	Ag20—S9	2.570 (3)
Ag4—Ag17	2.973 (4)	Ag20—O16	2.474 (7)
Ag4—S11	2.413 (4)	Ag20—O29	2.166 (7)
Ag4—S13	2.611 (4)	Ag21—Ag22	3.1890 (13)
Ag4—O23	2.440 (10)	Ag21—S6	2.526 (3)
Ag5—Ag8^{i}	3.341 (4)	Ag21—S9	2.586 (3)
Ag5—Ag17^{i}	2.847 (2)	Ag21—O18	2.422 (8)
Ag5—Ag28	2.940 (2)	Ag21—O33	2.380 (8)
Ag5—Ag29	2.846 (2)	Ag22—Ag23	2.8496 (12)
Ag5—S1	2.425 (3)	Ag22—Ag32	3.1659 (12)
Ag5—S10^{i}	2.515 (4)	Ag22—Ag33	3.1015 (12)
Ag5—O5^{i}	2.258 (10)	Ag22—S7	2.498 (3)
Ag6—Ag30	3.3164 (19)	Ag22—S9	2.656 (3)
Ag6—S1	2.536 (3)	Ag22—O28	2.269 (7)
Ag6—S4	2.569 (3)	Ag22—O33	2.502 (9)
Ag7—Ag21	3.0118 (19)	Ag23—Ag33	2.9538 (12)
Ag7—Ag27	3.358 (3)	Ag23—S8	2.526 (3)
Ag7—S4	2.603 (4)	Ag23—S9	2.644 (3)
Ag7—S6	2.478 (3)	Ag23—O27	2.292 (7)

Ag7—O35	2.49 (2)	Ag24—Ag25	3.3313 (12)
Ag8—Ag5^{i}	3.342 (4)	Ag24—S5	2.395 (3)
Ag8—Ag17	3.182 (3)	Ag24—S12	2.410 (3)
Ag8—Ag18	3.023 (3)	Ag25—Ag26	3.0076 (12)
Ag8—S10	2.604 (6)	Ag25—Ag27	3.1382 (12)
Ag8—S11	2.304 (5)	Ag25—S5	2.483 (3)
Ag8—O20	2.387 (10)	Ag25—S6	2.460 (3)
Ag9—Ag33	3.084 (11)	Ag25—O30	2.412 (8)
Ag9—S8	2.392 (11)	Ag26—Ag27	3.1627 (12)
Ag9—S10	2.623 (12)	Ag26—S2	2.454 (3)
Ag9—O7	2.319 (14)	Ag26—S5	2.482 (3)
Ag9—O9	2.497 (11)	Ag26—O17	2.332 (7)
Ag10—Ag14	3.3569 (11)	Ag27—Ag28	3.0342 (12)
Ag10—O11^{i}	2.429 (7)	Ag27—S2	2.533 (3)
Ag10—O14	2.329 (7)	Ag27—S6	2.482 (3)
Ag10—O17	2.499 (7)	Ag27—O31	2.501 (8)
Ag11—Ag12	2.8602 (13)	Ag28—Ag29	3.1031 (13)
Ag11—Ag13	3.0932 (11)	Ag28—S1	2.505 (3)
Ag11—Ag30^{i}	3.2824 (12)	Ag28—S2	2.549 (3)
Ag11—S3^{i}	2.553 (3)	Ag28—O32	2.361 (9)
Ag11—S13	2.586 (3)	Ag29—S2	2.452 (4)
Ag11—O22	2.294 (8)	Ag29—S10^{i}	2.498 (4)
Ag11—O36^{i}	2.427 (16)	Ag29—O4^{i}	2.337 (7)
Ag12—Ag13	2.9071 (12)	Ag29—O9^{i}	2.494 (7)
Ag12—S13	2.668 (3)	Ag30—Ag31	3.0254 (11)
Ag12—S14	2.532 (3)	Ag30—Ag32	3.0090 (12)
Ag12—O21	2.272 (8)	Ag30—S3	2.502 (3)
Ag13—Ag14	2.9799 (11)	Ag30—S4	2.463 (3)
Ag13—S3^{i}	2.429 (3)	Ag30—O3^{i}	2.487 (8)
Ag13—S14	2.447 (3)	Ag30—O36	2.341 (18)
Ag13—O6	2.321 (7)	Ag31—Ag32	2.9270 (12)
Ag14—Ag24	3.3094 (14)	Ag31—S3	2.481 (3)
Ag14—S5	2.717 (3)	Ag31—S7	2.533 (3)
Ag14—S14	2.465 (3)	Ag31—O2^{i}	2.375 (7)
Ag14—O11^{i}	2.290 (7)	Ag31—O10	2.384 (8)
Ag14—O14	2.400 (7)	Ag32—S4	2.464 (3)
Ag15—Ag16	2.9194 (14)	Ag32—S7	2.481 (3)
Ag15—Ag24	2.9457 (13)	Ag32—O18	2.529 (7)
Ag15—S12	2.460 (3)	Ag32—O33	2.592 (10)
Ag15—S14	2.546 (3)	Ag33—S7	2.467 (3)
Ag15—O8	2.406 (7)	Ag33—S8	2.449 (3)
Ag15—O23	2.362 (8)	Ag33—O15	2.299 (7)
Ag16—Ag18	2.9849 (14)		

O2^{i}—Ag1—O10	91.1 (3)	O13—Ag18—O26	88.8 (3)
O4—Ag2—O9	84.2 (2)	O26—Ag18—S8	87.1 (2)
O7—Ag2—O4	82.5 (2)	S9—Ag19—O26	104.4 (2)
O7—Ag2—O9	81.0 (2)	S12—Ag19—S9	143.94 (10)
S13—Ag3—S1^{i}	142.12 (17)	S12—Ag19—O26	105.2 (2)
O3—Ag3—S1^{i}	85.3 (2)	O13—Ag19—S9	114.89 (19)
O3—Ag3—S13	117.8 (3)	O13—Ag19—S12	85.64 (19)
S11—Ag4—S13	148.6 (2)	O13—Ag19—O26	89.2 (3)
S11—Ag4—O23	105.3 (3)	O16—Ag20—S9	83.49 (17)
O23—Ag4—S13	105.9 (2)	O29—Ag20—S9	139.7 (2)
S1—Ag5—S10^{i}	157.7 (3)	O29—Ag20—O16	130.2 (3)
O5^{i}—Ag5—S1	109.7 (3)	S6—Ag21—S9	142.09 (9)
O5^{i}—Ag5—S10^{i}	92.6 (2)	O18—Ag21—S6	87.4 (2)
S1—Ag6—S4	144.84 (11)	O18—Ag21—S9	104.0 (2)
S6—Ag7—S4	154.4 (2)	O33—Ag21—S6	122.1 (3)
S6—Ag7—O35	108.9 (5)	O33—Ag21—S9	95.2 (3)
O35—Ag7—S4	86.4 (5)	O33—Ag21—O18	84.4 (3)
S11—Ag8—S10	159.7 (3)	S7—Ag22—S9	141.94 (9)
S11—Ag8—O20	93.9 (3)	S7—Ag22—O33	101.9 (2)
O20—Ag8—S10	105.58 (19)	O28—Ag22—S7	118.3 (2)
S8—Ag9—S10	123.9 (4)	O28—Ag22—S9	95.2 (2)
S8—Ag9—O9	140.8 (5)	O28—Ag22—O33	96.6 (3)
O7—Ag9—S8	113.7 (5)	O33—Ag22—S9	90.7 (2)
O7—Ag9—S10	93.5 (4)	S8—Ag23—S9	142.56 (9)
O7—Ag9—O9	83.6 (4)	O27—Ag23—S8	110.8 (2)
O9—Ag9—S10	87.6 (4)	O27—Ag23—S9	104.2 (2)
O11^{i}—Ag10—O17	83.5 (2)	S5—Ag24—S12	168.89 (11)
O14—Ag10—O11^{i}	86.9 (2)	S6—Ag25—S5	158.98 (10)
O14—Ag10—O17	83.3 (2)	O30—Ag25—S5	104.66 (19)
S3^{i}—Ag11—S13	139.79 (9)	O30—Ag25—S6	96.11 (19)
O22—Ag11—S3^{i}	103.4 (3)	S2—Ag26—S5	142.60 (10)
O22—Ag11—S13	110.4 (3)	O17—Ag26—S2	105.54 (18)
O22—Ag11—O36^{i}	105.6 (6)	O17—Ag26—S5	106.23 (19)
O36^{i}—Ag11—S3^{i}	91.6 (4)	S6—Ag27—S2	151.60 (9)
O36^{i}—Ag11—S13	99.6 (5)	S6—Ag27—O31	103.9 (2)
S14—Ag12—S13	144.12 (9)	O31—Ag27—S2	104.0 (2)
O21—Ag12—S13	95.0 (2)	S1—Ag28—S2	154.45 (10)
O21—Ag12—S14	118.6 (2)	O32—Ag28—S1	106.3 (2)
S3^{i}—Ag13—S14	149.07 (9)	O32—Ag28—S2	98.2 (3)
O6—Ag13—S3^{i}	100.5 (2)	S2—Ag29—S10^{i}	139.57 (10)
O6—Ag13—S14	109.2 (2)	S2—Ag29—O9^{i}	116.15 (18)
S14—Ag14—S5	112.23 (9)	O4^{i}—Ag29—S2	105.52 (19)
O11^{i}—Ag14—S5	88.7 (2)	O4^{i}—Ag29—S10^{i}	105.60 (19)

O11^{i}—Ag14—S14	154.8 (2)	O4^{i}—Ag29—O9^{i}	87.2 (2)
O11^{i}—Ag14—O14	88.5 (2)	O9^{i}—Ag29—S10^{i}	90.52 (19)
O14—Ag14—S5	90.98 (18)	S4—Ag30—S3	159.41 (9)
O14—Ag14—S14	104.42 (17)	S4—Ag30—O3^{i}	99.3 (2)
S12—Ag15—S14	139.56 (10)	O3^{i}—Ag30—S3	88.1 (2)
O8—Ag15—S12	115.2 (2)	O36—Ag30—S3	95.0 (4)
O8—Ag15—S14	81.8 (2)	O36—Ag30—S4	104.6 (4)
O23—Ag15—S12	123.4 (2)	O36—Ag30—O3^{i}	86.7 (5)
O23—Ag15—S14	90.4 (2)	S3—Ag31—S7	138.07 (9)
O23—Ag15—O8	91.5 (3)	O2^{i}—Ag31—S3	107.90 (18)
S11—Ag16—S12	137.16 (10)	O2^{i}—Ag31—S7	105.42 (19)
O24—Ag16—S11	99.8 (3)	O2^{i}—Ag31—O10	89.5 (2)
O24—Ag16—S12	100.2 (3)	O10—Ag31—S3	109.4 (2)
O25—Ag16—S11	112.6 (3)	O10—Ag31—S7	95.5 (2)
O25—Ag16—S12	94.1 (3)	S4—Ag32—S7	164.19 (10)
O25—Ag16—O24	112.2 (3)	S4—Ag32—O18	100.4 (2)
O5—Ag17—S13	81.7 (2)	S4—Ag32—O33	94.4 (2)
O19—Ag17—S13	148.2 (2)	S7—Ag32—O18	89.25 (19)
O19—Ag17—O5	129.7 (3)	S7—Ag32—O33	99.9 (2)
S11—Ag18—S8	149.83 (11)	O18—Ag32—O33	78.1 (3)
S11—Ag18—O13	112.21 (19)	S8—Ag33—S7	142.91 (9)
S11—Ag18—O26	119.3 (2)	O15—Ag33—S7	100.51 (19)
O13—Ag18—S8	80.40 (18)	O15—Ag33—S8	115.20 (19)
Symmetry code: (i) −*x*+2, −*y*+1, −*z*+1.			
SD/Ag66c			
Ag1—Ag2	2.727 (9)	Ag33—S11	2.487 (4)
Ag1—Ag4	2.783 (8)	Ag33—S19	2.507 (4)
Ag1—O27	2.414 (11)	Ag34—Ag51	3.087 (2)
Ag1—O30	2.442 (10)	Ag34—O54	2.330 (12)
Ag2—Ag3	2.802 (9)	Ag34—O62	2.334 (11)
Ag2—Ag6	2.694 (10)	Ag34—S11	2.619 (5)
Ag2—O6	2.51 (3)	Ag34—S18	2.602 (5)
Ag2—O11	2.240 (13)	Ag35—Ag36	2.861 (2)
Ag3—Ag4	2.711 (8)	Ag35—Ag52	2.919 (2)
Ag3—O7	2.46 (2)	Ag35—O31	2.339 (11)
Ag3—O18	2.274 (12)	Ag35—S10	2.517 (4)
Ag3—O22	2.514 (11)	Ag35—S18	2.504 (5)
Ag4—Ag5	2.740 (8)	Ag36—Ag37	2.871 (2)
Ag4—Ag6	2.818 (9)	Ag36—O28	2.461 (10)
Ag4—O25	2.208 (12)	Ag36—O63	2.138 (17)
Ag5—Ag6	2.637 (7)	Ag36—S10	2.535 (5)
Ag5—O15	2.483 (12)	Ag37—Ag38	2.996 (2)
Ag5—O17	2.353 (11)	Ag37—Ag53	3.126 (2)

Ag6—O12	2.499 (12)	Ag37—O26	2.449 (10)
Ag6—O36	2.279 (12)	Ag37—O49	2.280 (17)
Ag7—Ag8	3.326 (11)	Ag37—S10	2.721 (5)
Ag7—Ag15	3.294 (9)	Ag37—S17	2.481 (5)
Ag7—Ag27	2.993 (10)	Ag38—Ag39	2.939 (2)
Ag7—Ag28	3.057 (9)	Ag38—Ag54	3.242 (3)
Ag7—S21	2.512 (9)	Ag38—O50	2.332 (15)
Ag7—S28	2.546 (10)	Ag38—O65	2.418 (17)
Ag8—Ag27	3.370 (3)	Ag38—S9	2.778 (5)
Ag8—O1	2.51 (3)	Ag38—S17	2.673 (5)
Ag8—O15	2.405 (11)	Ag39—Ag40	2.825 (3)
Ag8—S22	2.451 (7)	Ag39—O24	2.431 (10)
Ag8—S28	2.491 (6)	Ag39—O66	2.265 (19)
Ag9—Ag15	3.120 (2)	Ag39—S9	2.524 (5)
Ag9—Ag16	2.969 (3)	Ag39—S16	2.754 (5)
Ag9—O1	2.58 (3)	Ag40—Ag41	2.927 (2)
Ag9—O12	2.334 (11)	Ag40—Ag55	2.935 (2)
Ag9—S27	2.445 (5)	Ag40—O23	2.566 (10)
Ag9—S28	2.484 (6)	Ag40—O48	2.169 (15)
Ag10—Ag11	3.071 (2)	Ag40—S16	2.536 (5)
Ag10—Ag17	3.253 (2)	Ag41—Ag56	3.339 (2)
Ag10—Ag18	2.967 (2)	Ag41—O19	2.390 (11)
Ag10—O36	2.319 (9)	Ag41—S8	2.495 (5)
Ag10—S26	2.440 (5)	Ag41—S16	2.502 (5)
Ag10—S27	2.446 (5)	Ag42—Ag57	3.006 (2)
Ag11—Ag20	3.095 (2)	Ag42—O46	2.339 (13)
Ag11—O2	2.28 (3)	Ag42—O70	2.357 (14)
Ag11—O29	2.396 (10)	Ag42—S8	2.591 (5)
Ag11—S25	2.566 (5)	Ag42—S15	2.601 (5)
Ag11—S26	2.482 (5)	Ag43—Ag44	3.076 (3)
Ag12—Ag21	3.101 (2)	Ag43—Ag58	2.956 (2)
Ag12—Ag22	2.978 (2)	Ag43—O20	2.426 (10)
Ag12—O25	2.362 (11)	Ag43—S14	2.464 (5)
Ag12—S24	2.460 (6)	Ag43—S15	2.478 (5)
Ag12—S25	2.469 (5)	Ag44—Ag45	2.906 (5)
Ag13—Ag14	3.160 (2)	Ag44—O14	2.566 (11)
Ag13—Ag23	3.075 (2)	Ag44—O71	2.30 (3)
Ag13—Ag24	3.014 (2)	Ag44—S14	2.464 (6)
Ag13—O21	2.336 (10)	Ag45—Ag46	3.133 (4)
Ag13—S23	2.453 (5)	Ag45—Ag59	3.327 (3)
Ag13—S24	2.483 (5)	Ag45—O13	2.428 (12)
Ag14—Ag26	3.041 (3)	Ag45—O41	2.55 (2)
Ag14—O3	2.31 (3)	Ag45—O42	2.33 (3)

Ag14—O17	2.368 (11)	Ag45—S21	2.499 (6)
Ag14—S22	2.584 (6)	Ag46—Ag47	3.133 (3)
Ag14—S23	2.501 (5)	Ag46—Ag59	3.346 (3)
Ag15—Ag16	3.083 (3)	Ag46—Ag60	2.904 (3)
Ag15—Ag29	3.352 (3)	Ag46—O13	2.547 (11)
Ag15—O10	2.559 (11)	Ag46—S2	2.439 (6)
Ag15—O40	2.55 (2)	Ag46—S13	2.400 (6)
Ag15—S20	2.442 (6)	Ag47—Ag48	3.090 (3)
Ag15—S28	2.502 (6)	Ag47—Ag60	3.326 (3)
Ag16—Ag17	3.275 (2)	Ag47—O37	2.53 (3)
Ag16—Ag30	3.183 (3)	Ag47—S3	2.528 (7)
Ag16—Ag31	3.356 (3)	Ag47—S13	2.441 (7)
Ag16—S20	2.465 (5)	Ag48—Ag49	2.943 (3)
Ag16—S27	2.502 (5)	Ag48—Ag61	2.902 (3)
Ag17—Ag18	2.887 (2)	Ag48—S3	2.445 (5)
Ag17—Ag31	2.998 (2)	Ag48—S12	2.460 (5)
Ag17—O58	2.50 (2)	Ag49—Ag50	3.168 (2)
Ag17—O59	2.324 (14)	Ag49—Ag61	3.132 (3)
Ag17—S19	2.583 (5)	Ag49—O56	2.31 (2)
Ag17—S27	2.585 (6)	Ag49—S4	2.492 (5)
Ag18—Ag33	2.937 (2)	Ag49—S12	2.555 (5)
Ag18—O60	2.286 (12)	Ag50—Ag51	2.979 (2)
Ag18—O61	2.574 (11)	Ag50—Ag62	3.076 (3)
Ag18—S19	2.604 (5)	Ag50—O33	2.541 (11)
Ag18—S26	2.505 (5)	Ag50—S4	2.456 (6)
Ag19—Ag20	2.977 (2)	Ag50—S11	2.435 (5)
Ag19—Ag34	2.9702 (18)	Ag51—O31	2.482 (10)
Ag19—O32	2.482 (11)	Ag51—O53	2.354 (13)
Ag19—O61	2.336 (12)	Ag51—S5	2.562 (5)
Ag19—S18	2.482 (4)	Ag51—S11	2.487 (4)
Ag19—S26	2.548 (4)	Ag52—Ag53	2.861 (2)
Ag20—Ag21	3.144 (2)	Ag52—Ag63	3.039 (2)
Ag20—Ag36	3.300 (2)	Ag52—O52	2.271 (13)
Ag20—O28	2.581 (11)	Ag52—O53	2.563 (12)
Ag20—S18	2.414 (5)	Ag52—S5	2.511 (5)
Ag20—S25	2.475 (5)	Ag52—S10	2.665 (5)
Ag21—Ag22	3.062 (2)	Ag53—Ag63	3.054 (2)
Ag21—Ag36	2.986 (2)	Ag53—O49	2.554 (17)
Ag21—O64	2.427 (16)	Ag53—O51	2.278 (14)
Ag21—S17	2.472 (5)	Ag53—S6	2.519 (6)
Ag21—S25	2.496 (5)	Ag53—S10	2.549 (5)
Ag22—Ag38	3.316 (2)	Ag54—Ag55	3.053 (2)
Ag22—O24	2.430 (11)	Ag54—Ag64	3.031 (3)

Ag22—S17	2.467 (5)	Ag54—O26	2.405 (11)
Ag22—S24	2.530 (6)	Ag54—S6	2.539 (7)
Ag23—Ag24	2.8636 (19)	Ag54—S9	2.467 (5)
Ag23—Ag39	3.091 (2)	Ag55—Ag56	3.086 (2)
Ag23—O67	2.277 (15)	Ag55—Ag64	3.187 (2)
Ag23—S16	2.564 (5)	Ag55—O47	2.426 (17)
Ag23—S24	2.531 (6)	Ag55—S7	2.516 (5)
Ag24—Ag41	2.937 (2)	Ag55—S9	2.480 (5)
Ag24—O68	2.300 (15)	Ag56—Ag57	2.960 (2)
Ag24—O69	2.544 (13)	Ag56—Ag65	3.075 (3)
Ag24—S16	2.619 (5)	Ag56—O23	2.564 (11)
Ag24—S23	2.510 (5)	Ag56—S7	2.466 (5)
Ag25—Ag26	2.988 (2)	Ag56—S8	2.430 (5)
Ag25—Ag42	3.069 (2)	Ag57—O20	2.473 (11)
Ag25—O19	2.481 (11)	Ag57—O45	2.341 (12)
Ag25—O69	2.365 (14)	Ag57—S1	2.552 (5)
Ag25—S15	2.487 (5)	Ag57—S8	2.495 (5)
Ag25—S23	2.572 (5)	Ag58—Ag59	2.866 (2)
Ag26—Ag27	3.193 (3)	Ag58—Ag66	2.979 (2)
Ag26—Ag43	3.233 (2)	Ag58—O44	2.302 (15)
Ag26—O14	2.514 (12)	Ag58—O45	2.502 (13)
Ag26—S15	2.425 (5)	Ag58—S1	2.529 (5)
Ag26—S22	2.461 (6)	Ag58—S14	2.602 (6)
Ag27—Ag44	2.999 (3)	Ag59—Ag66	3.261 (2)
Ag27—O72	2.06 (3)	Ag59—O41	2.42 (2)
Ag27—S21	2.570 (6)	Ag59—O43	2.304 (14)
Ag27—S22	2.472 (6)	Ag59—S2	2.562 (6)
Ag28—Ag29	3.147 (3)	Ag59—S14	2.514 (6)
Ag28—Ag45	3.010 (3)	Ag60—O6	2.45 (3)
Ag28—O10	2.426 (11)	Ag60—O11	2.316 (10)
Ag28—O40	2.52 (2)	Ag60—S2	2.456 (6)
Ag28—S13	2.489 (7)	Ag60—S3	2.505 (6)
Ag28—S21	2.589 (6)	Ag61—O35	2.399 (11)
Ag29—Ag47	3.204 (3)	Ag61—S3	2.474 (6)
Ag29—O38	2.33 (3)	Ag61—S4	2.460 (6)
Ag29—O39	2.38 (2)	Ag62—Ag63	3.145 (2)
Ag29—S13	2.639 (6)	Ag62—O5	2.48 (3)
Ag29—S20	2.629 (6)	Ag62—O30	2.376 (10)
Ag30—Ag31	3.031 (3)	Ag62—S4	2.585 (5)
Ag30—Ag48	2.878 (3)	Ag62—S5	2.493 (5)
Ag30—O9	2.504 (11)	Ag63—O27	2.308 (9)
Ag30—S12	2.512 (6)	Ag63—S5	2.442 (5)
Ag30—S20	2.437 (6)	Ag63—S6	2.478 (6)

Ag31—Ag32	2.901 (3)	Ag64—O22	2.345 (11)
Ag31—O34	2.431 (11)	Ag64—S6	2.438 (6)
Ag31—O57	2.237 (19)	Ag64—S7	2.459 (6)
Ag31—S12	2.628 (5)	Ag65—Ag66	3.178 (2)
Ag31—S19	2.756 (5)	Ag65—O7	2.52 (3)
Ag32—Ag33	2.921 (2)	Ag65—O18	2.379 (11)
Ag32—Ag49	2.930 (2)	Ag65—S1	2.466 (5)
Ag32—O33	2.429 (11)	Ag65—S7	2.543 (5)
Ag32—O55	2.18 (2)	Ag66—O16	2.326 (10)
Ag32—S19	2.558 (5)	Ag66—S1	2.436 (5)
Ag33—Ag50	3.299 (2)	Ag66—S2	2.469 (6)
Ag33—O32	2.405 (10)		
O27—Ag1—O30	86.1 (4)	O57—Ag31—S12	114.1 (6)
O11—Ag2—O6	84.6 (8)	O57—Ag31—S19	112.4 (6)
O17—Ag5—O15	83.3 (4)	O63—Ag36—S10	130.8 (5)
O36—Ag6—O12	83.8 (4)	O26—Ag37—S10	96.8 (3)
S21—Ag7—S28	149.1 (6)	O26—Ag37—S17	85.2 (3)
O15—Ag8—O1	89.2 (6)	O49—Ag37—O26	97.1 (6)
O15—Ag8—S22	101.0 (3)	O49—Ag37—S10	92.6 (4)
O15—Ag8—S28	102.1 (3)	O49—Ag37—S17	134.3 (4)
S22—Ag8—O1	129.6 (7)	S17—Ag37—S10	132.71 (16)
S22—Ag8—S28	135.6 (2)	O50—Ag38—O65	107.7 (6)
S28—Ag8—O1	88.2 (7)	O50—Ag38—S9	88.4 (5)
O1A—Ag9—O1	34.7 (9)	O50—Ag38—S17	113.7 (5)
O1A—Ag9—S27	86.4 (7)	O65—Ag38—S9	109.7 (5)
O1A—Ag9—S28	120.0 (7)	O65—Ag38—S17	89.5 (5)
O12—Ag9—O1	83.5 (6)	S17—Ag38—S9	145.37 (15)
O12—Ag9—S27	111.2 (3)	O24—Ag39—S9	85.5 (3)
O12—Ag9—S28	104.4 (3)	O24—Ag39—S16	95.3 (3)
S27—Ag9—O1	119.4 (6)	O66—Ag39—O24	99.4 (6)
S27—Ag9—S28	137.22 (18)	O66—Ag39—S9	140.2 (5)
S28—Ag9—O1	86.8 (6)	O66—Ag39—S16	96.2 (5)
O36—Ag10—S26	114.9 (3)	S9—Ag39—S16	122.78 (17)
O36—Ag10—S27	103.1 (3)	O48—Ag40—O23	135.4 (5)
S26—Ag10—S27	140.12 (16)	O48—Ag40—S16	129.3 (4)
O2—Ag11—O29	91.7 (7)	S16—Ag40—O23	83.0 (3)
O2—Ag11—S25	114.1 (8)	O19—Ag41—S8	83.2 (3)
O2—Ag11—S26	117.2 (8)	O19—Ag41—S16	122.9 (3)
O29—Ag11—S25	95.1 (3)	S8—Ag41—S16	149.63 (17)
O29—Ag11—S26	109.2 (3)	O46—Ag42—O70	110.3 (5)
S26—Ag11—S25	121.42 (17)	O46—Ag42—S8	107.0 (4)
O25—Ag12—S24	107.9 (3)	O46—Ag42—S15	99.4 (4)
O25—Ag12—S25	102.6 (3)	O70—Ag42—S8	99.9 (3)

S24—Ag12—S25	140.63 (18)	O70—Ag42—S15	100.1 (4)
O21—Ag13—S23	116.1 (3)	S8—Ag42—S15	138.64 (15)
O21—Ag13—S24	98.6 (3)	O20—Ag43—S14	125.1 (3)
S23—Ag13—S24	143.61 (16)	O20—Ag43—S15	83.0 (3)
O3—Ag14—O17	90.1 (7)	S14—Ag43—S15	150.90 (18)
O3—Ag14—S22	124.7 (7)	O71—Ag44—O14	125.9 (9)
O3—Ag14—S23	105.9 (7)	O71—Ag44—S14	131.0 (9)
O17—Ag14—S22	95.9 (3)	S14—Ag44—O14	85.8 (3)
O17—Ag14—S23	108.4 (3)	O13—Ag45—O41	103.1 (6)
S23—Ag14—S22	123.54 (18)	O13—Ag45—S21	84.6 (3)
O40—Ag15—O10	81.1 (6)	O42—Ag45—O13	153.8 (8)
S20—Ag15—O10	98.1 (3)	O42—Ag45—O41	50.8 (9)
S20—Ag15—O40	102.5 (6)	O42—Ag45—S21	121.4 (7)
S20—Ag15—S28	156.33 (19)	S21—Ag45—O41	166.7 (5)
S28—Ag15—O10	86.5 (3)	S2—Ag46—O13	86.9 (3)
S28—Ag15—O40	101.1 (6)	S13—Ag46—O13	103.7 (3)
S20—Ag16—S27	160.7 (2)	S13—Ag46—S2	164.5 (2)
O58—Ag17—S19	114.5 (6)	S3—Ag47—O37	106.0 (5)
O58—Ag17—S27	90.8 (6)	S13—Ag47—O37	106.2 (5)
O59—Ag17—O58	93.2 (6)	S13—Ag47—S3	147.8 (2)
O59—Ag17—S19	117.6 (4)	S3—Ag48—S12	167.3 (2)
O59—Ag17—S27	95.8 (4)	O56—Ag49—S4	106.5 (6)
S19—Ag17—S27	135.19 (15)	O56—Ag49—S12	99.8 (6)
O60—Ag18—O61	102.0 (4)	S4—Ag49—S12	153.62 (19)
O60—Ag18—S19	96.8 (4)	S4—Ag50—O33	90.8 (3)
O60—Ag18—S26	113.5 (4)	S11—Ag50—O33	103.6 (3)
O61—Ag18—S19	101.4 (3)	S11—Ag50—S4	164.65 (17)
S26—Ag18—O61	86.8 (3)	O31—Ag51—S5	82.2 (3)
S26—Ag18—S19	146.31 (15)	O31—Ag51—S11	101.9 (3)
O32—Ag19—S26	83.0 (3)	O53—Ag51—O31	92.2 (4)
O61—Ag19—O32	92.3 (4)	O53—Ag51—S5	89.3 (3)
O61—Ag19—S18	123.4 (3)	O53—Ag51—S11	121.9 (3)
O61—Ag19—S26	91.1 (3)	S11—Ag51—S5	147.98 (17)
S18—Ag19—O32	102.9 (3)	O52—Ag52—O53	104.1 (5)
S18—Ag19—S26	144.17 (16)	O52—Ag52—S5	118.6 (6)
S18—Ag20—O28	102.6 (3)	O52—Ag52—S10	97.2 (5)
S18—Ag20—S25	166.68 (18)	O53—Ag52—S10	101.7 (4)
S25—Ag20—O28	90.0 (3)	S5—Ag52—O53	86.0 (3)
O64—Ag21—S17	107.5 (5)	S5—Ag52—S10	140.58 (14)
O64—Ag21—S25	93.7 (5)	O51—Ag53—O49	101.7 (6)
S17—Ag21—S25	158.53 (17)	O51—Ag53—S6	102.7 (5)
O24—Ag22—S17	112.9 (3)	O51—Ag53—S10	108.8 (5)
O24—Ag22—S24	87.1 (3)	S6—Ag53—O49	101.5 (5)

S17—Ag22—S24	156.67 (19)	S6—Ag53—S10	143.10 (15)
O67—Ag23—S16	109.3 (5)	S10—Ag53—O49	90.6 (5)
O67—Ag23—S24	104.7 (6)	O26—Ag54—S6	86.9 (3)
S24—Ag23—S16	141.40 (16)	O26—Ag54—S9	117.3 (3)
O68—Ag24—O69	104.8 (5)	S9—Ag54—S6	153.87 (19)
O68—Ag24—S16	96.3 (5)	O47—Ag55—S7	92.6 (5)
O68—Ag24—S23	114.7 (5)	O47—Ag55—S9	110.3 (5)
O69—Ag24—S16	101.5 (3)	S9—Ag55—S7	157.05 (17)
S23—Ag24—O69	87.8 (3)	S7—Ag56—O23	90.5 (3)
S23—Ag24—S16	144.35 (15)	S8—Ag56—O23	103.0 (3)
O19—Ag25—S15	102.9 (3)	S8—Ag56—S7	166.39 (19)
O19—Ag25—S23	82.5 (3)	O20—Ag57—S1	83.6 (3)
O69—Ag25—O19	91.6 (4)	O20—Ag57—S8	103.0 (3)
O69—Ag25—S15	123.7 (3)	O45—Ag57—O20	93.7 (4)
O69—Ag25—S23	90.4 (3)	O45—Ag57—S1	88.8 (4)
S15—Ag25—S23	144.86 (17)	O45—Ag57—S8	121.5 (3)
S15—Ag26—O14	104.0 (3)	S8—Ag57—S1	147.97 (16)
S15—Ag26—S22	163.36 (19)	O44—Ag58—O45	103.0 (5)
S22—Ag26—O14	90.4 (3)	O44—Ag58—S1	107.7 (5)
O72—Ag27—S21	100.5 (9)	O44—Ag58—S14	100.8 (5)
O72—Ag27—S22	108.5 (9)	O45—Ag58—S1	85.8 (3)
S22—Ag27—S21	150.3 (2)	O45—Ag58—S14	104.6 (4)
O10—Ag28—O40	84.5 (5)	S1—Ag58—S14	146.55 (16)
O10—Ag28—S13	88.2 (3)	O41—Ag59—S2	96.4 (6)
O10—Ag28—S21	107.4 (3)	O41—Ag59—S14	104.7 (7)
O40—Ag28—S21	98.6 (6)	O43—Ag59—O41	95.7 (7)
S13—Ag28—O40	118.5 (7)	O43—Ag59—S2	97.1 (5)
S13—Ag28—S21	141.1 (2)	O43—Ag59—S14	116.8 (4)
O38—Ag29—O39	91.8 (9)	S14—Ag59—S2	137.22 (17)
O38—Ag29—S13	95.3 (7)	O6—Ag60—S2	92.0 (7)
O38—Ag29—S20	105.7 (7)	O6—Ag60—S3	120.2 (7)
O39—Ag29—S13	104.7 (6)	O11—Ag60—O6	84.4 (6)
O39—Ag29—S20	92.7 (6)	O11—Ag60—S2	112.8 (3)
S20—Ag29—S13	152.29 (16)	O11—Ag60—S3	103.6 (3)
O9—Ag30—S12	105.6 (3)	S2—Ag60—S3	133.50 (19)
S20—Ag30—O9	86.4 (3)	O35—Ag61—S3	107.1 (3)
S20—Ag30—S12	163.42 (19)	O35—Ag61—S4	101.0 (3)
O34—Ag31—S12	80.1 (3)	S4—Ag61—S3	140.52 (19)
O34—Ag31—S19	92.8 (3)	O5—Ag62—S4	84.4 (7)
O57—Ag31—O34	134.6 (8)	O5—Ag62—S5	144.3 (7)
S12—Ag31—S19	120.07 (16)	O30—Ag62—O5	84.4 (6)
O33—Ag32—S19	85.1 (3)	O30—Ag62—S4	93.2 (3)
O55—Ag32—O33	139.2 (7)	O30—Ag62—S5	110.7 (3)

O55—Ag32—S19	132.2 (6)	S5—Ag62—S4	124.85 (18)
O32—Ag33—S11	83.0 (3)	O27—Ag63—S5	114.9 (3)
O32—Ag33—S19	123.9 (3)	O27—Ag63—S6	99.8 (3)
S11—Ag33—S19	149.84 (17)	S5—Ag63—S6	143.65 (16)
O54—Ag34—O62	107.4 (4)	O22—Ag64—S6	107.7 (3)
O54—Ag34—S11	99.0 (4)	O22—Ag64—S7	101.6 (3)
O54—Ag34—S18	103.4 (4)	S6—Ag64—S7	137.98 (19)
O62—Ag34—S11	98.8 (4)	O7—Ag65—S7	85.5 (7)
O62—Ag34—S18	106.2 (4)	O18—Ag65—O7	86.5 (6)
S18—Ag34—S11	139.30 (14)	O18—Ag65—S1	111.1 (3)
O31—Ag35—S10	123.4 (3)	O18—Ag65—S7	96.7 (3)
O31—Ag35—S18	85.2 (3)	S1—Ag65—O7	141.3 (7)
S18—Ag35—S10	141.75 (17)	S1—Ag65—S7	123.98 (18)
O28—Ag36—S10	84.8 (3)	O16—Ag66—S1	115.7 (3)
O63—Ag36—O28	142.0 (6)	O16—Ag66—S2	103.8 (3)
S1—Ag66—S2	138.53 (17)		
SD/Ag66d			
Ag1—Ag14	3.152 (3)	Ag8—Ag16	2.974 (3)
Ag1—O7^{i}	2.299 (12)	Ag8—O3	2.284 (15)
Ag1—S2	2.388 (6)	Ag8—S8	2.405 (6)
Ag1—S8^{i}	2.437 (5)	Ag9—Ag10	3.017 (4)
Ag2—Ag3	2.632 (6)	Ag9—Ag16	3.114 (4)
Ag2—Ag5^{i}	3.028 (7)	Ag9—O19	2.43 (4)
Ag2—O10^{i}	2.561 (14)	Ag9—S8	2.469 (6)
Ag2—O14	1.63 (3)	Ag10—Ag16	3.282 (4)
Ag2—S1	2.687 (7)	Ag10—O1	2.27 (4)
Ag2—S2	2.676 (7)	Ag10—O5	2.385 (12)
Ag3—Ag4	3.246 (7)	Ag10—S1^{i}	2.943 (8)
Ag3—Ag15	2.896 (5)	Ag10—S6	2.590 (6)
Ag3—O10^{i}	2.515 (14)	Ag11—Ag11^{ii}	3.268 (5)
Ag3—O14	2.35 (3)	Ag11—Ag12	2.942 (3)
Ag3—S2	2.529 (7)	Ag11—Ag13	3.125 (3)
Ag3—S3	2.421 (6)	Ag11—S5	2.406 (8)
Ag4—Ag5	3.305 (6)	Ag11—S6	2.512 (6)
Ag4—Ag6	3.213 (6)	Ag12—Ag13	2.999 (3)
Ag4—Ag12	3.210 (5)	Ag12—O16	2.36 (4)
Ag4—S3	2.437 (7)	Ag12—S4	2.560 (7)
Ag4—S4	2.623 (8)	Ag12—S6	2.557 (6)
Ag5—Ag2^{i}	3.028 (7)	Ag13—Ag13^{ii}	3.355 (4)
Ag5—Ag6	2.802 (6)	Ag13—O6	2.325 (12)
Ag5—S1^{i}	2.706 (7)	Ag13—O11	2.517 (16)
Ag5—S3	2.414 (7)	Ag13—S4	2.457 (7)
Ag6—Ag10	2.899 (6)	Ag13—S5	2.454 (7)

Ag6—Ag12	2.873 (4)	Ag14—O9	2.354 (12)
Ag6—O8	2.392 (11)	Ag14—O12	2.49 (2)
Ag6—O17	2.21 (3)	Ag14—S2	2.502 (5)
Ag6—S1^{i}	2.627 (6)	Ag14—S4	2.496 (7)
Ag6—S6	2.848 (7)	Ag15—O15^{i}	2.54 (3)
Ag7—Ag7^{ii}	2.940 (7)	Ag15—O15	2.54 (3)
Ag7—Ag10	2.919 (6)	Ag15—S3	2.536 (6)
Ag7—Ag11	2.848 (5)	Ag15—S3^{i}	2.536 (6)
Ag7—Ag16	3.358 (4)	Ag16—Ag16^{ii}	3.071 (3)
Ag7—O4	2.188 (13)	Ag16—O2	2.36 (3)
Ag7—S6	2.471 (6)	Ag16—S7	2.479 (5)
Ag7—S7	2.496 (6)	Ag16—S8	2.525 (5)
O7^{i}—Ag1—S2	109.0 (4)	O1—Ag10—S1^{i}	106.8 (10)
O7^{i}—Ag1—S8^{i}	102.5 (4)	O1—Ag10—S6	120.7 (10)
S2—Ag1—S8^{i}	142.66 (19)	O5—Ag10—S1^{i}	88.9 (3)
O10^{i}—Ag2—S1	100.9 (4)	O5—Ag10—S6	85.1 (3)
O10^{i}—Ag2—S2	79.5 (4)	S6—Ag10—S1^{i}	115.5 (2)
O14—Ag2—O10^{i}	102.1 (10)	S5—Ag11—S6	149.5 (3)
O14—Ag2—S1	128.3 (10)	O16—Ag12—S4	102.4 (9)
O14—Ag2—S2	104.3 (10)	O16—Ag12—S6	106.1 (8)
S2—Ag2—S1	125.1 (3)	S6—Ag12—S4	148.4 (2)
O10^{i}—Ag3—S2	83.2 (4)	O6—Ag13—O11	82.0 (5)
O14—Ag3—O10^{i}	85.6 (8)	O6—Ag13—S4	104.6 (3)
O14—Ag3—S2	90.2 (7)	O6—Ag13—S5	113.2 (3)
O14—Ag3—S3	118.9 (7)	S4—Ag13—O11	111.0 (4)
S3—Ag3—O10^{i}	109.4 (4)	S5—Ag13—O11	91.6 (4)
S3—Ag3—S2	148.4 (3)	S5—Ag13—S4	138.3 (2)
S3—Ag4—S4	153.6 (3)	O9—Ag14—O12	88.1 (5)
S3—Ag5—S1^{i}	137.7 (3)	O9—Ag14—S2	107.1 (3)
O8—Ag6—S1^{i}	85.0 (3)	O9—Ag14—S4	99.2 (3)
O8—Ag6—S6	95.2 (4)	O12—Ag14—S2	103.6 (4)
O17—Ag6—O8	117.0 (10)	S4—Ag14—O12	121.1 (4)
O17—Ag6—S1^{i}	120.5 (9)	S4—Ag14—S2	128.5 (2)
O17—Ag6—S6	114.4 (9)	O15^{i}—Ag15—O15	102.8 (10)
S1^{i}—Ag6—S6	117.6 (2)	S3—Ag15—O15^{i}	97.1 (6)
O4—Ag7—S6	117.2 (5)	S3^{i}—Ag15—O15^{i}	102.1 (6)
O4—Ag7—S7	86.0 (6)	S3—Ag15—O15	102.1 (6)
S6—Ag7—S7	155.1 (2)	S3—Ag15—S3^{i}	149.1 (3)
O3—Ag8—S8	106.77 (14)	O2—Ag16—S7	102.1 (9)
S8^{ii}—Ag8—S8	143.1 (3)	O2—Ag16—S8	99.5 (9)
O19—Ag9—S8	102.4 (9)	S7—Ag16—S8	156.35 (18)
O1—Ag10—O5	136.3 (12)		
Symmetry codes: (i) −*x*+2, −*y*+1, *z*; (ii) *x*, *y*, −*z*+1.			

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