

Electronic Supporting Information

Regulating the assembly and expansion of the silver cluster from the Ag_{37} to Ag_{46} nanowheel driven by heteroanions

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Experiment details

The silver precursor [i PrSAg] $_n$ ¹ and the macrocyclic ligand *p*-phenyl-thiacalix[4]arene (H₄PTC4A)² were prepared according to the reported literature. Silver benzoate (PhCOOAg, 99%) was procured from Shanghai Titan Scientific Co., Ltd. Other chemicals and solvents involved in the syntheses were of analytical grade and used without further purification. Infrared spectra were recorded on a Bruker Tensor II spectrophotometer (Bruker Optics GmbH, Ettlingen, Germany) utilizing a single attenuated total reflectance (ATR) accessory covering a wavenumber range from 500 to 4000 cm⁻¹. The final spectra were the average of 32 scans accumulated using Bruker's Opus software 8.1, taken at 4 cm⁻¹ resolution. The samples were measured under the same mechanical force pushing the samples in contact with the diamond window. Powder X-ray diffraction (PXRD) analyses were carried out on a microcrystalline powder using a Rigaku Oxford Diffraction XtaLAB Synergy diffractometer using Cu radiation ($\lambda = 1.54184 \text{ \AA}$). The PXRD patterns were processed with the *CrysAlis^{Pro}* software suite³ using the Powder function. UV-Vis absorption spectra were recorded on a Thermo Scientific Evolution 220 UV-visible spectrophotometer. Mass spectra (MS) were recorded on a Bruker impact II high definition mass spectrometer, quadrupole and time-of-flight (Q/TOF) modules. Typical measurement conditions are as follows: end plate offset = -400 V; dry gas = 3 L min⁻¹, nebulizer = 0.3 bar, capillary voltage = 3500 V, sample flow rate = 180 $\mu\text{L h}^{-1}$. The data analyses of mass spectra were performed based on the isotope distribution patterns using Compass Data Analysis software (Version 4.4).

X-ray Crystallography

Single crystals of **Ag37** and **Ag46** with appropriate dimensions were selected under an optical microscope and rapidly coated with high vacuum grease (Dow Corning Corporation) to prevent decomposition. The single-crystal X-ray diffraction (SCXRD) data of **Ag37** and **Ag46** were recorded at 173 K and 100 K, respectively, on a Rigaku Oxford Diffraction XtaLAB Synergy diffractometer equipped with Rigaku Hypix detector and an Oxford Cryosystems CryostreamPlus 800 open-flow N₂ cooling device. A Cu K α radiation ($\lambda = 1.54184 \text{ \AA}$) from PhotonJet micro-focus X-ray sources was used for the measurement. The diffraction images were processed and scaled using the *CrysAlis^{Pro}* software.³ Both structures were solved using the charge-flipping algorithm, as implemented in the program *SUPERFLIP*⁴ and refined by full-matrix least-squares techniques against F_o^2 using the SHELXL program⁵ through the OLEX2 interface.⁶ 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 PLATON⁷ to ensure that no additional symmetry could be applied to the models. Pertinent crystallographic data collection and refinement parameters are collated in [Table S1](#). Selected bond lengths and angles are collated in [Table S6](#).

Dye adsorption measurements

Cationic dyes of methylene blue (MB) and rhodamine B (RhB), and anionic dye of methyl orange (MO) were used to evaluate the adsorption performance of the freshly prepared **Ag46**. In brief, the sample of **Ag46** (15 mg) was added to 5 mL aqueous solutions containing different dyes, followed by stirring at 1500 rpm in darkness at room temperature. The UV-Vis absorption spectra of the solutions were collected at different time intervals. The adsorption efficiency of **Ag46** was determined using the following equation:

$$\text{adsorption efficiency} = 1 - \frac{C_t}{C_o} \times 100\% = 1 - \frac{A_t}{A_o} \times 100\%$$

where C_o and C_t , A_o and A_t correspond to the concentration and absorbance of dyes before and after adsorption.

Molecular Docking Studies

Molecular docking studies were conducted using HEX 8.0.0 software with the following parameters: correlation type = shape only; grid dimension = 0.6; FFT mode = three-dimensional (3D); ligand range = 180; receptor range = 180; distance range = 40; twist range = 360. Mercury 2021.3.0 software was used to generate PDB (Protein Data Bank) from the crystal structure of **Ag46**. The coordinates of MB and RhB were taken from internet sources as mol files and converted to PDB files using Mercury 2021.3.0 software. It was envisaged that the coordinated CH₃CN in the cavity of *p*-phenyl-thiacalix[4]arene would exchange with solvent molecules. Therefore, CH₃CN was removed in order to better understand the interactions of **Ag46** with dyes. Later, the generated PDB files were used for molecular docking studies. Discovery Studio 2021 software was used to modify the structure and visualize the noncovalent interaction between **Ag46** and dyes.

Synthesis

Synthesis of Ag37

In a 10 mL glass reactor, H₄PTC4A (12 mg, 0.015 mmol), [ⁱPrSAg]_n (9.2 mg, 0.05 mmol) and NaCl (2 mg, 0.034 mmol) were added and dissolved in a CH₃CN/CH₂Cl₂/DMF solution (6.5 mL, v:v:v = 8:4:1). Then, PhCOOAg (22.9 mg, 0.1 mmol) were added to the above mixture after magnetically stirring for one hour at room temperature. After stirring for another three hours, the turbid solution is sealed in a 25 mL Teflon-lined reaction vessel and kept at 65 °C for 2000 minutes. The yellow-fusiform crystals suitable for X-ray diffraction analysis were obtained upon slowly cooling to room temperature (Yield: 5%; 1.3 mg). Selected IR peaks (cm⁻¹): 1677 (m), 1585 (m), 1421 (s), 1303 (m), 1238 (m), 1043 (w), 874 (m), 747 (s), 696 (s), 608 (s).

Synthesis of Ag46

The same synthetic procedure, as described for Ag37, was applied by adding (NH₄)₂Cr₂O₇ (7.3 mg, 0.029 mmol) and NaCl (2 mg, 0.034 mmol) simultaneously instead of NaCl. Dark-red cubic crystals were successfully obtained (Yield: 50%; 14 mg). In addition, a tenfold scale-up of the synthesis (Yield: 50%; 140 mg) can be obtained by increasing the amount of reactants: 0.15 mmol H₄PTC4A, 0.5 mmol [ⁱPrSAg]_n, 1 mmol PhCOOAg, 0.19 mmol (NH₄)₂Cr₂O₇, 0.051 mmol NaCl and 39 mL CH₃CN/CH₂Cl₂/DMF (v:v:v = 8:4:1). Selected IR peaks (cm⁻¹): 1584 (m), 1426 (s), 1308 (m), 1238 (m), 1145 (w), 1033 (w), 884 (w), 752 (s), 685 (s), 603 (s).

Figure S1: Microscope photographs of crystals of Ag37 and Ag46.

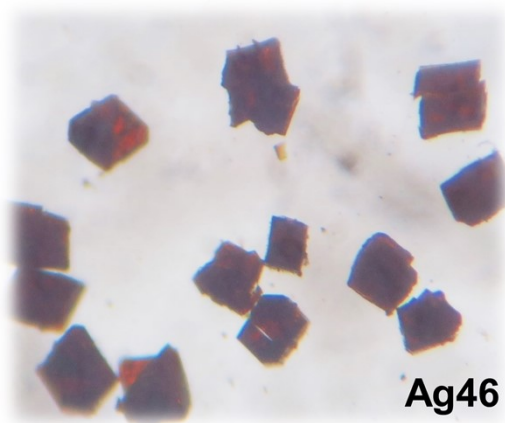
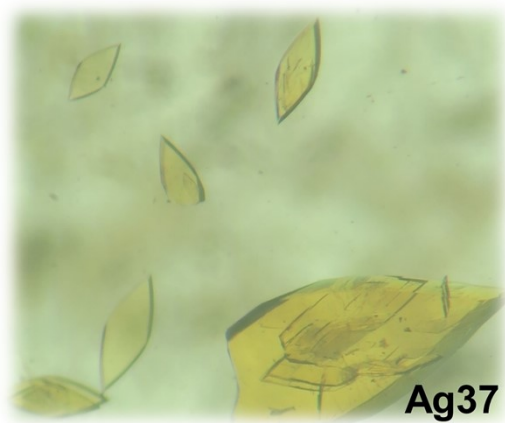


Figure S2: (a) and (b) Ag₂ (core)@Ag₃₅ (shell) skeletal structure of Ag₃₇ viewed along two orthogonal directions.

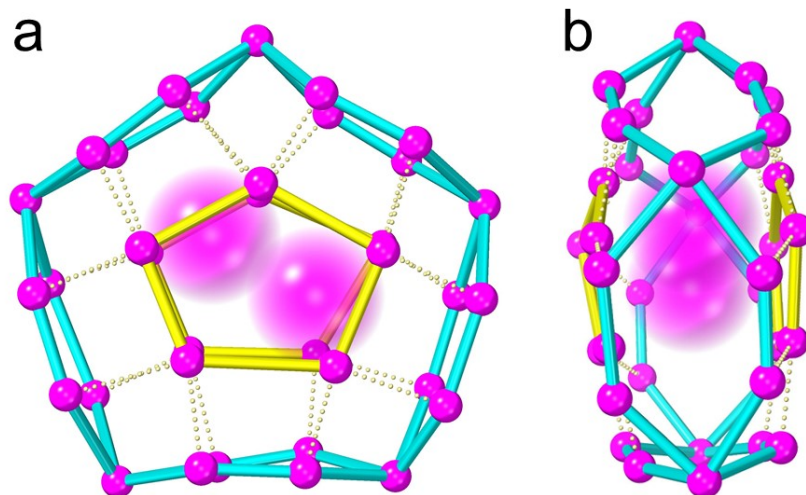


Figure S3: The coordinated solvent molecules (CH₃CN or DMF) present in each PTC4A⁴⁻ of Ag₃₇. Colour code: Ag, purple; Na, brown; O, red; S, yellow; Cl, green; C, gray; N, pale blue.

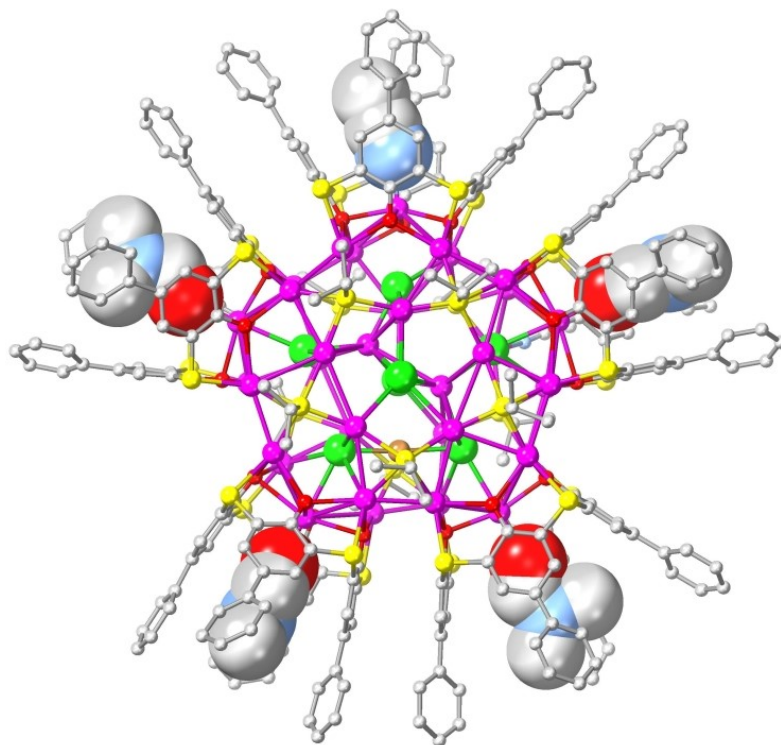


Figure S4: (a) and (b) The coordination and distribution of 10 i PrS $^-$ ligands on the $\text{Ag}_2@$ Ag_{35} skeleton of Ag_{37} viewed along two orthogonal directions. Colour code: Ag, purple and cyan; S, yellow; C, gray.

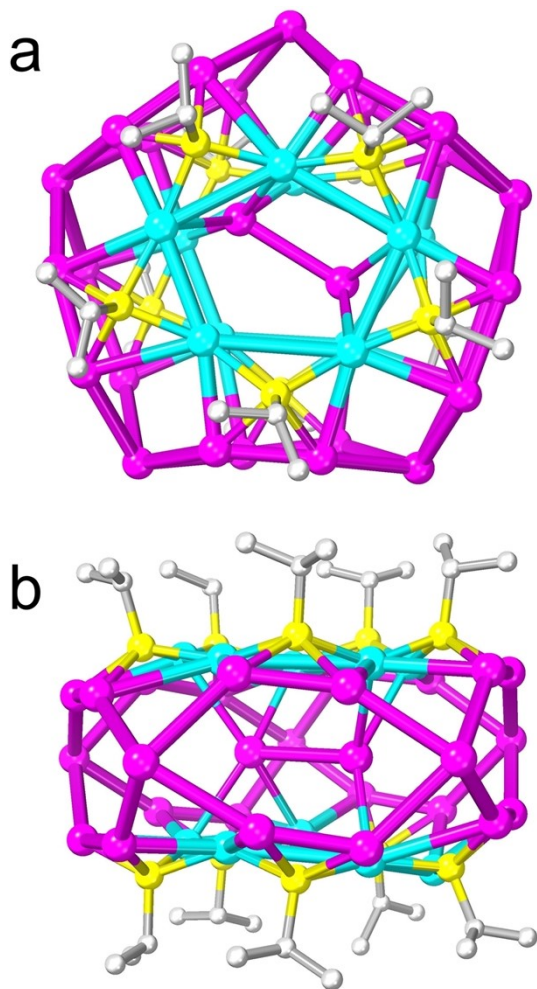


Figure S5: Extended structure of Ag37 showing self-assembly into a layered pattern along the [100] direction.

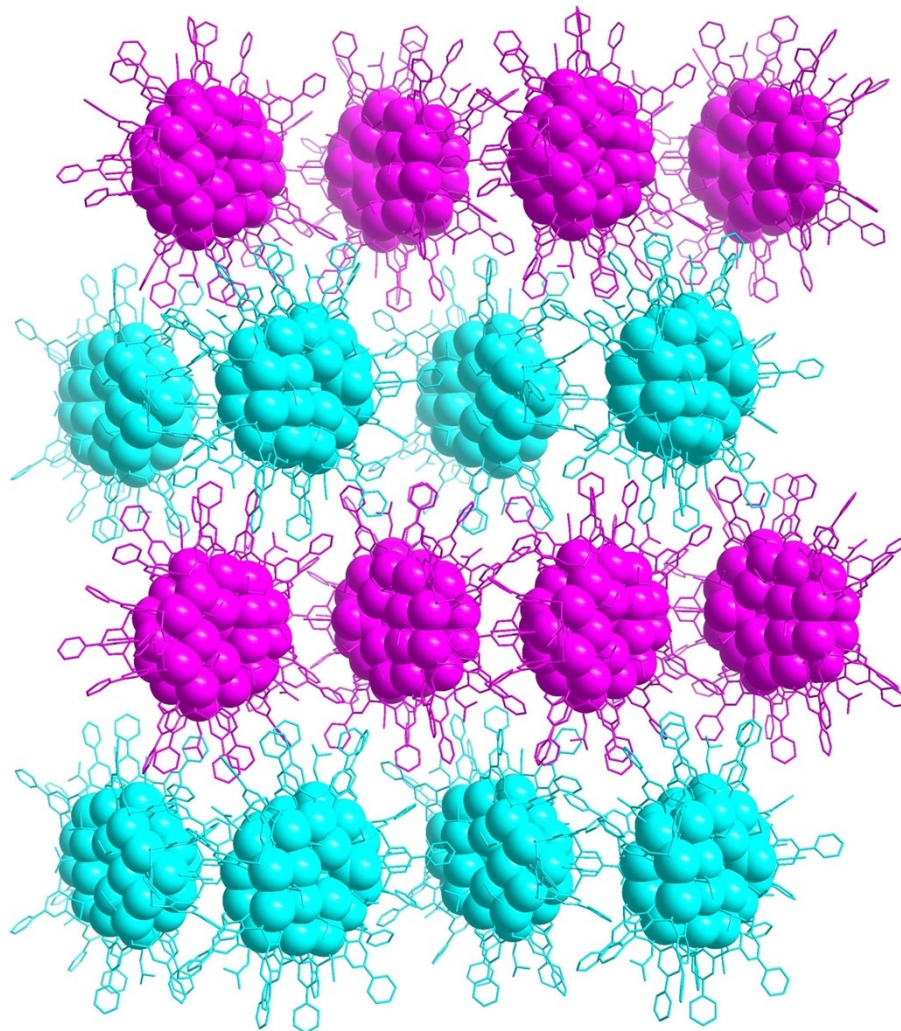


Figure S6: The coordinated CH_3CN molecules present in each PTC4A^{4-} of Ag_46 .

Colour code: Ag, purple; O, red; S, yellow; Cl, green; C, gray; N, pale blue; Cr, light orange.

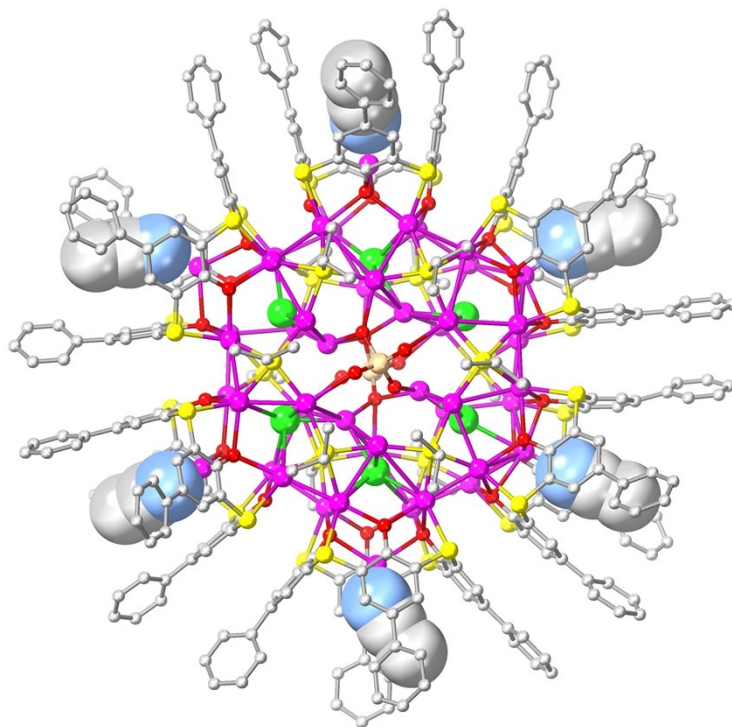


Figure S7: (a) and (b) The coordination and distribution of 12 *i*PrS⁻ ligands on the Ag₄@Ag₄₂ skeleton of Ag₄₆ viewed along two orthogonal directions. Colour code: Ag, purple and cyan; S, yellow; C, gray.

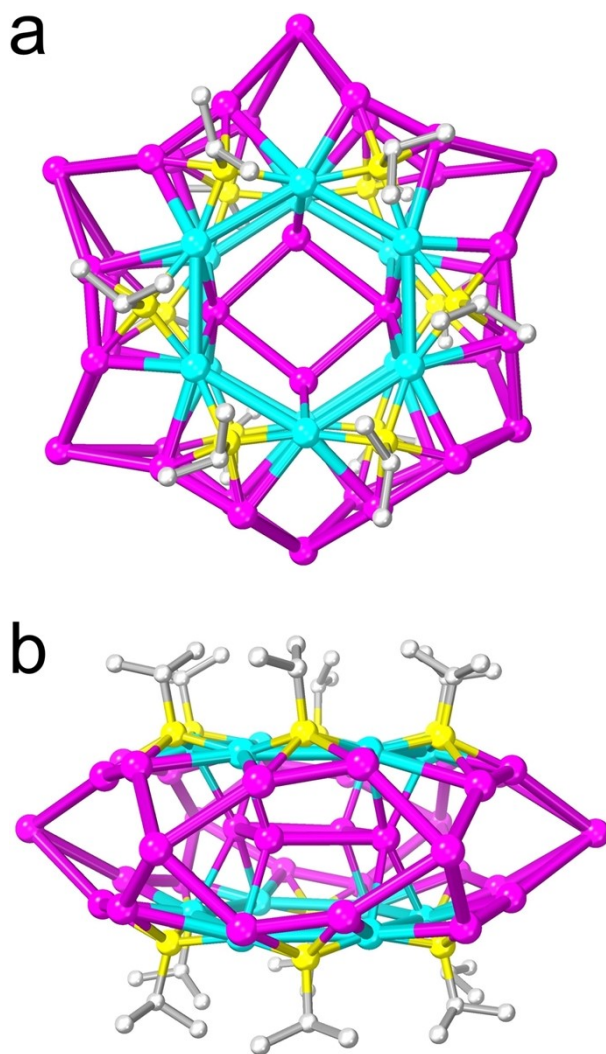


Figure S8: Extended structure of Ag46 showing self-assembly into a layered array along the [010] direction.

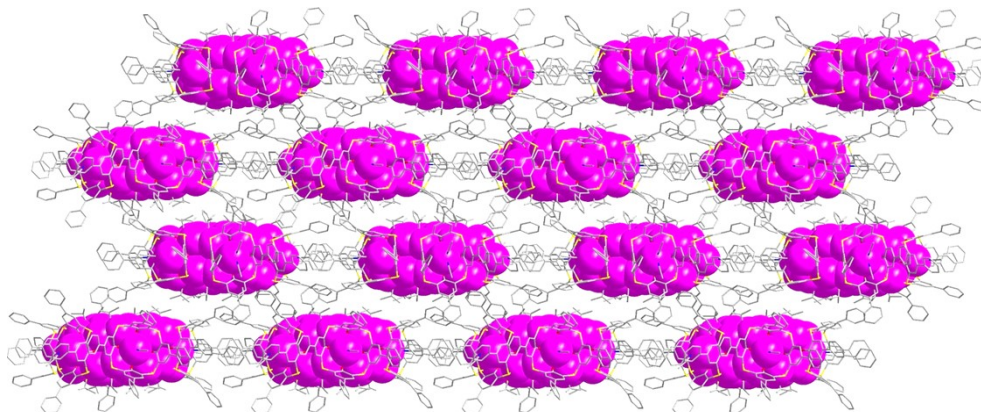


Figure S9: The structure and dimension of PTC4A⁴⁻ ligand. Colour code: C, gray;

O, red; S, yellow; H, white.

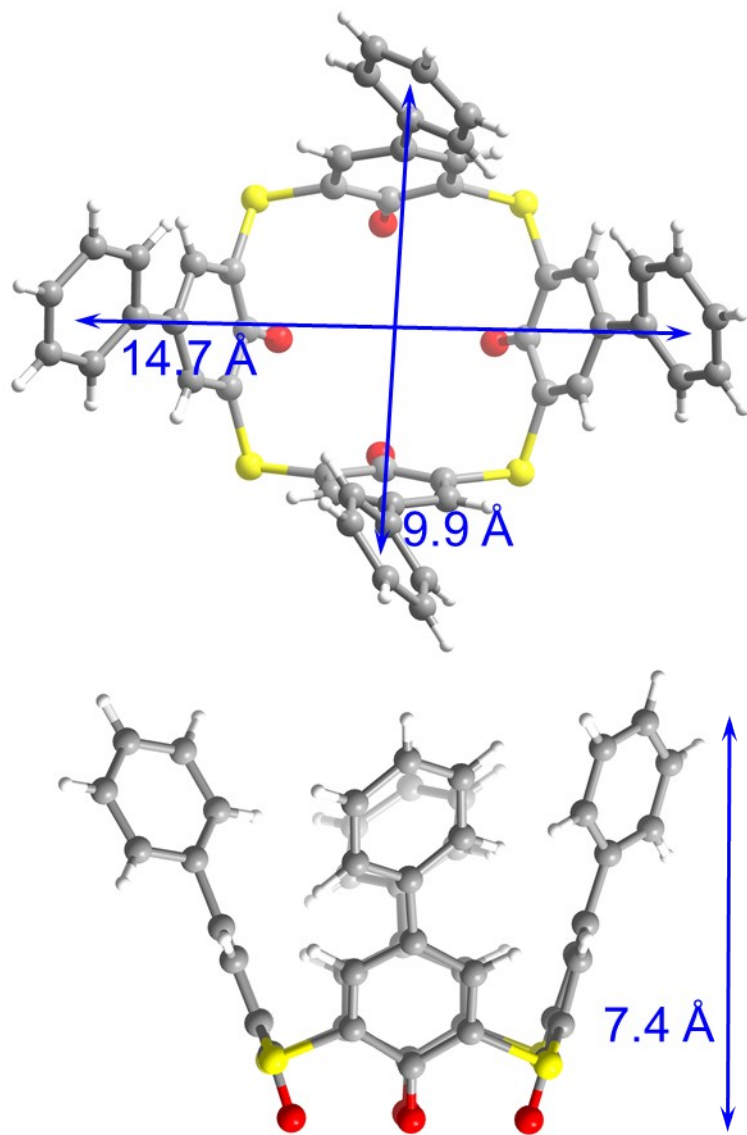


Figure S10: Electrostatic potential energy map for the PTC4A⁴⁻ ligand via Multiwfn software⁸.

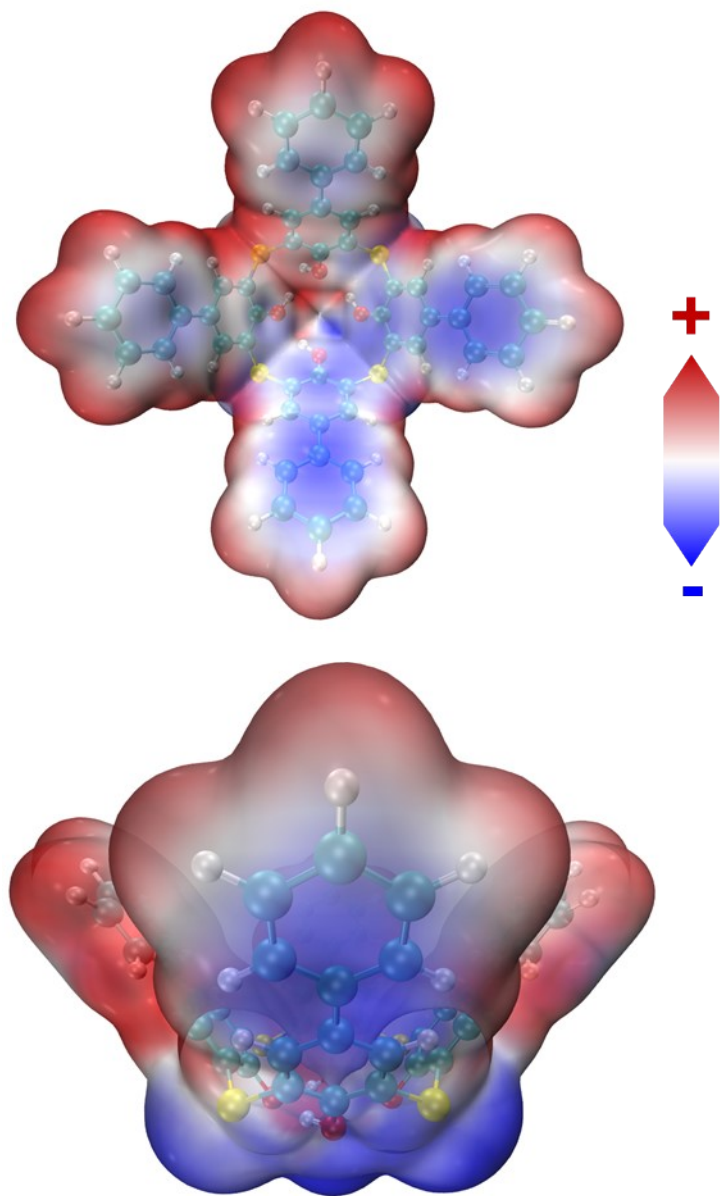


Figure S11: Visualization of the docked structure of MB and Ag46 using discovery studio software. The $\pi\cdots\pi$ interactions are shown with the dashed light blue line.

Colour code: Ag, purple; Cr, dark green; O, red; S, yellow; Cl, bright green; C, gray and sea blue; N, blue.

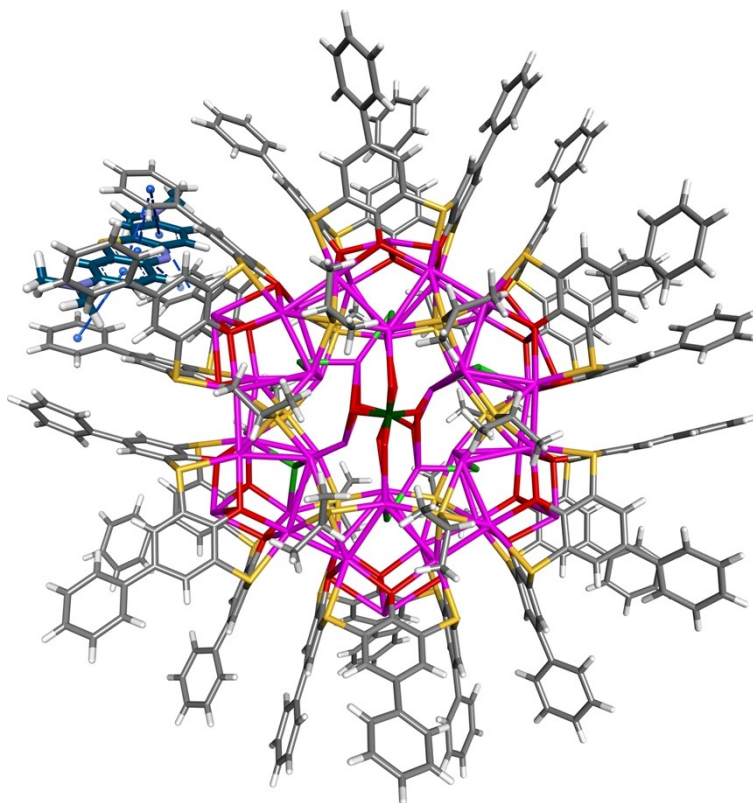


Figure S12: Visualization of docked structure of RhB and Ag46 using discovery studio software. The C-H $\cdots\pi$ and $\pi\cdots\pi$ interactions are shown with the dashed light blue line. Colour code: Ag, purple; Cr, dark green; O, red; S, yellow; Cl, bright green; C, gray and dark pink; N, blue.

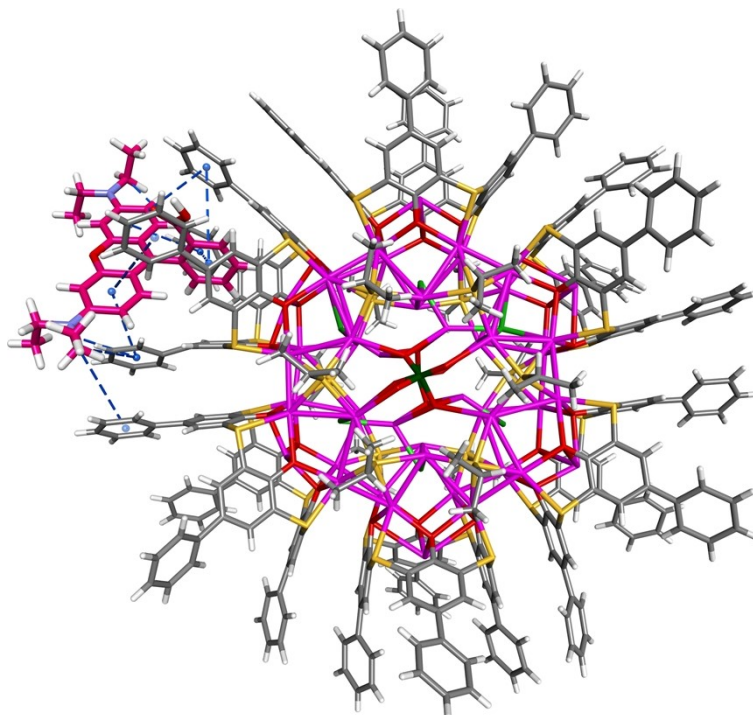
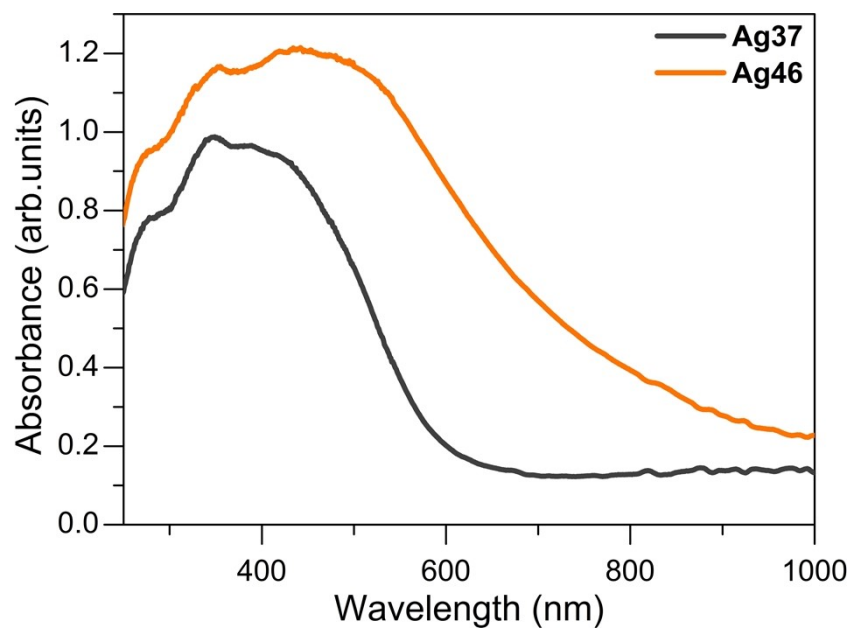
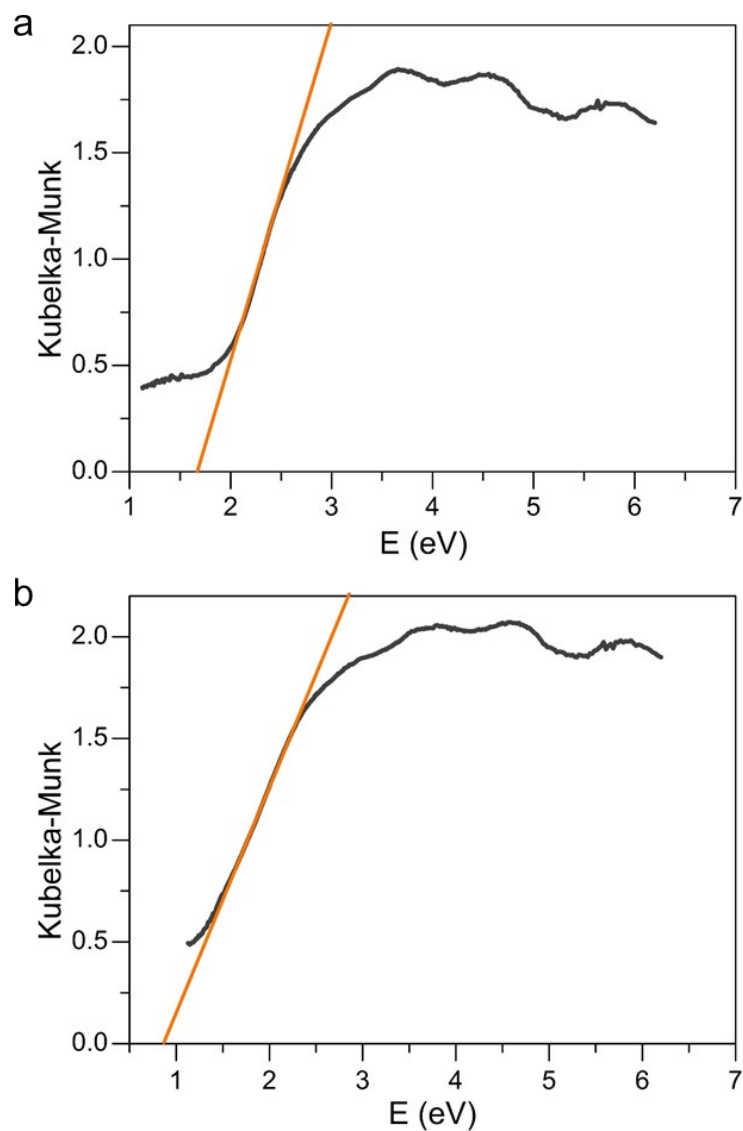


Figure S13: UV-Vis spectra of Ag37 and Ag46.



The solid-state UV-Vis absorption spectra of **Ag37** and **Ag46** were recorded at room temperature, and both exhibit similar shoulder peaks in the wavelength of 250-1000 nm. These two peaks at 350 nm and 420 nm can be attributed to ligand-based absorption and S 3p→Ag 5s electronic transition, respectively.⁹ Also, the absorption edge of **Ag46** is wider, which is consistent with the colors of the samples (yellow for **Ag37**; black-red for **Ag46**) (Fig. S1).

Figure S14: UV-Vis spectra of Kubelka-Munk function vs energy (eV) and Tauc plots of Ag37 (a) and Ag46 (b).



The band-gap of **Ag37** and **Ag46** were respectively calculated to be 1.66, and 0.87 eV based on the Kubelka-Munk function of $(\alpha h\nu)^{1/2} = \kappa(h\nu - E_g)$ (E_g is the band gap (eV), h is the Planck's constant (J.s), ν is the light frequency (s^{-1}), κ is the absorption constant and α is the absorption coefficient).^{10,11}

Figure S15: Compared PXRD patterns of Ag37.

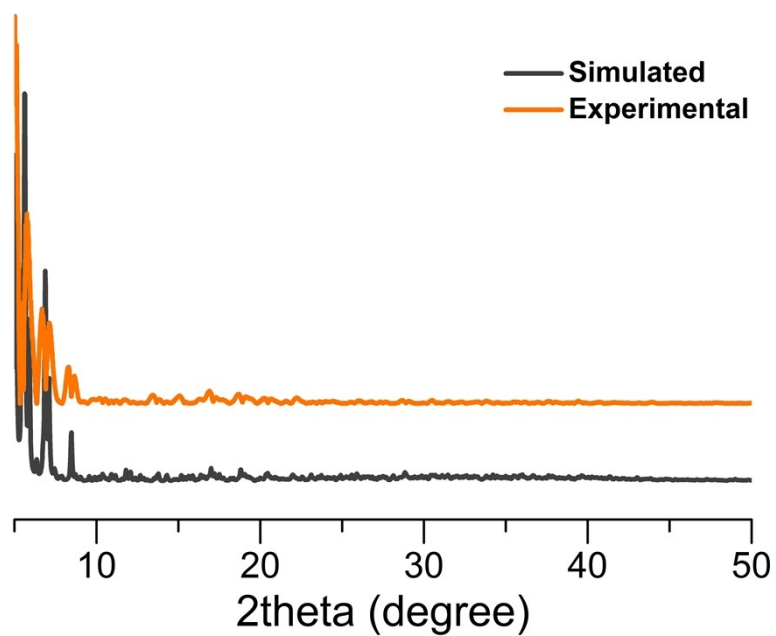


Figure S16: Compared PXRD patterns of Ag46.

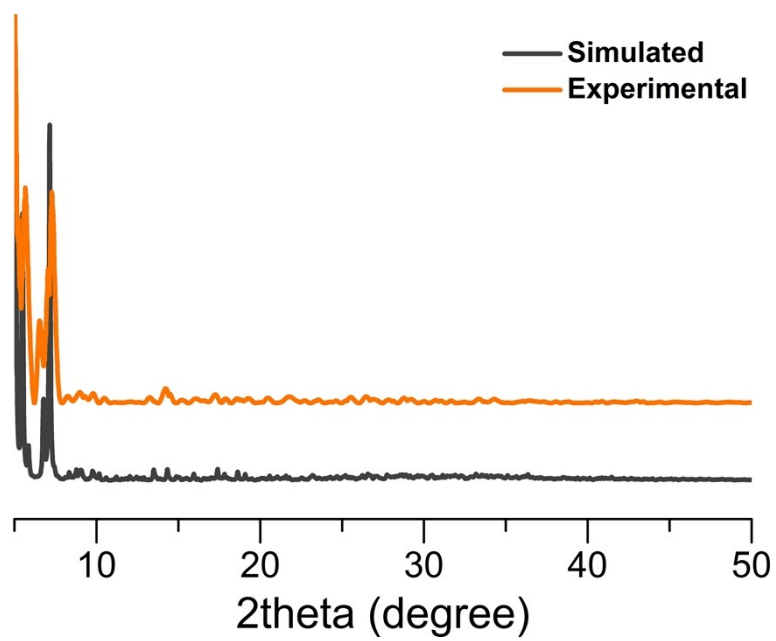


Figure S17: The IR spectrum of Ag37.

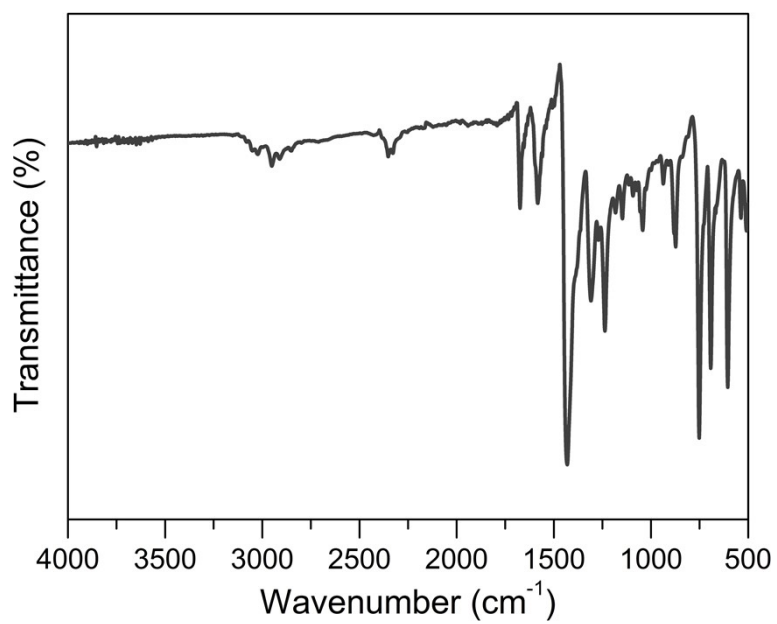


Figure S18: The IR spectrum of Ag46.

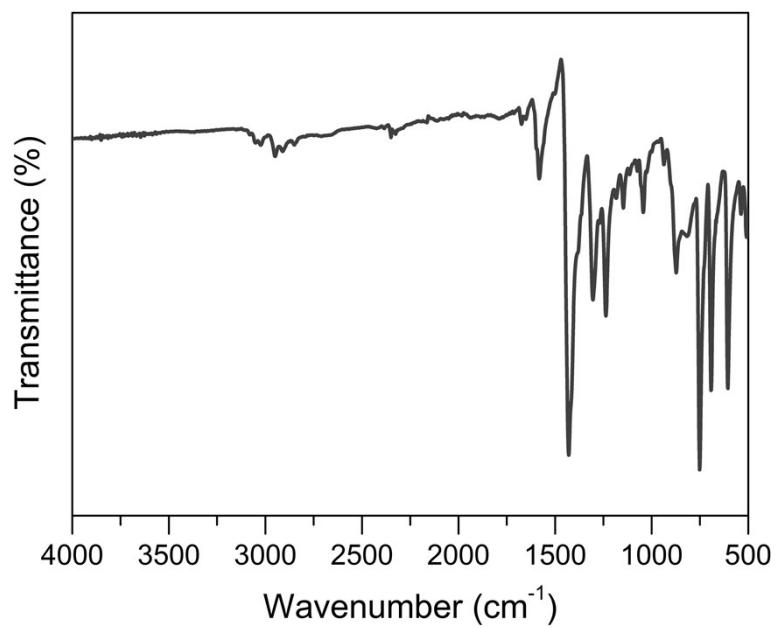


Figure S19: The crystal packing diagrams in unit cell of Ag37 viewed along *a* (a), *b* (b) and *c* (c) axis. Color code: purple, Ag; red, O; yellow, S; gray, C; blue, N; darkgreen, Na; green, Cl.

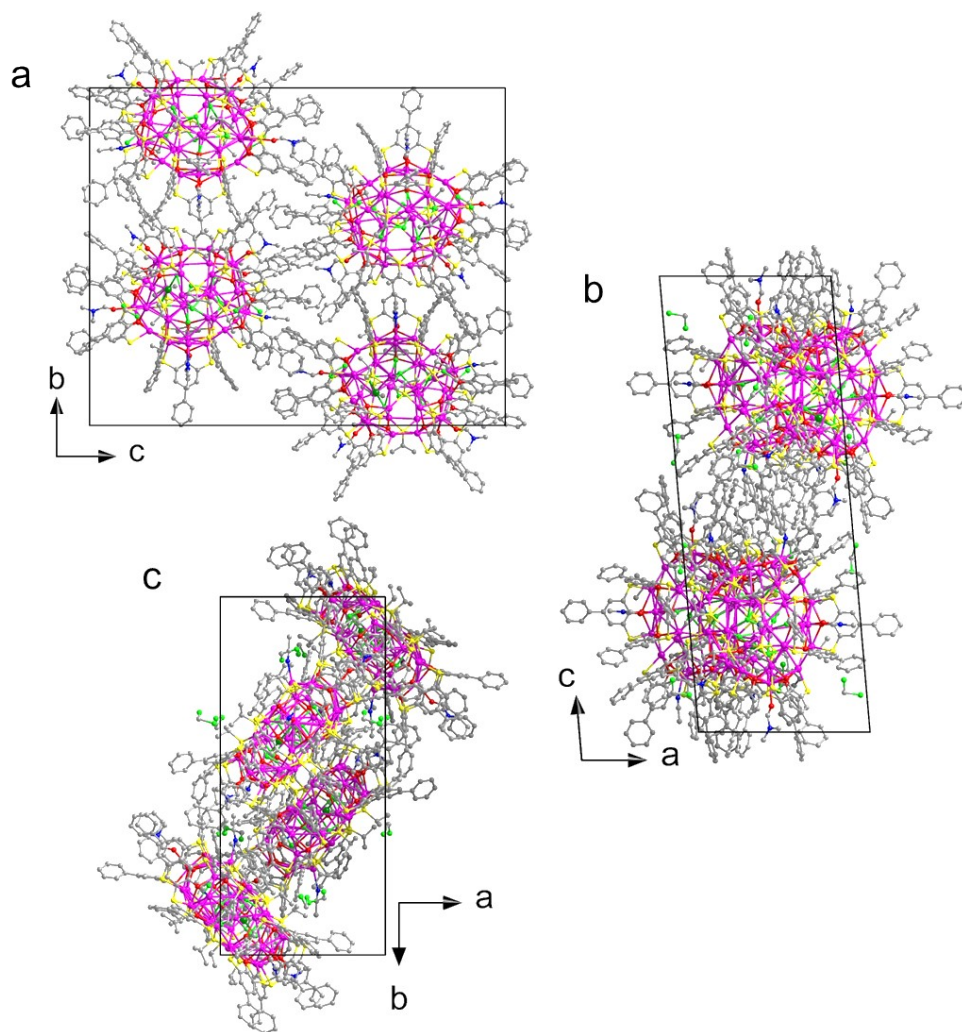


Figure S20: The crystal packing diagrams in unit cell of Ag46 viewed along a (a), b (b) and c (c) axis. Color code: purple, Ag; red, O; cyan, Cr; yellow, S; gray, C; blue, N; green, Cl.

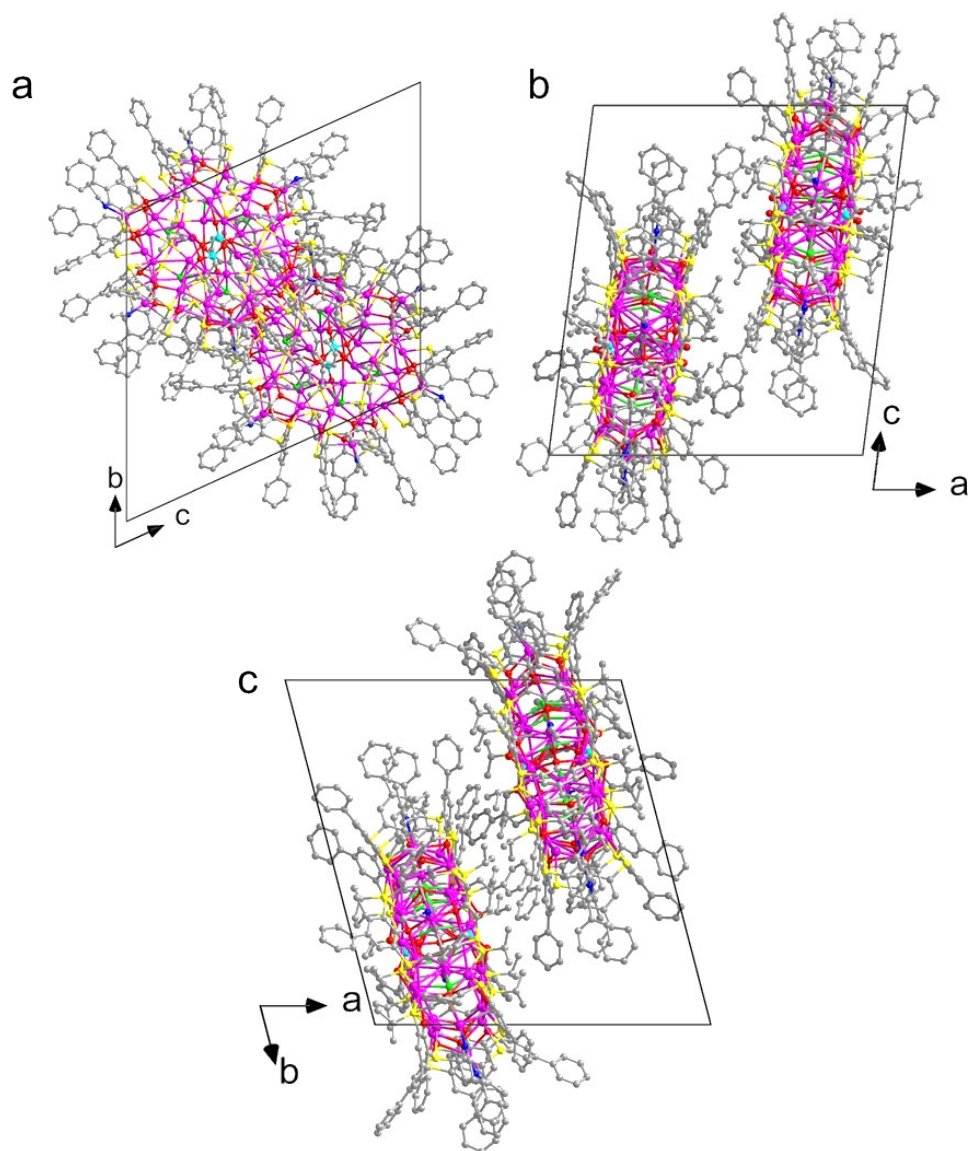


Table S1: Crystal data and structure refinements for Ag37 and Ag46.

Compound	Ag37	Ag46
Empirical formula	$C_{288}H_{248}Ag_{37}Cl_{11}N_6NaO_{24}S_3$ 0	$C_{336}H_{270}Ag_{46}Cl_6Cr_2N_6O_{32}S_{36}$
Formula weight	9542.84	11336.44
Temperature/K	173(2)	100.00(11)
Crystal system	monoclinic	triclinic
Space group	$P2_1/n$	$P-1$
a/Å	17.8704(4)	26.4405(4)
b/Å	38.6083(6)	30.6300(6)
c/Å	47.7137(5)	31.6049(6)
$\alpha/^\circ$	90	62.291(2)
$\beta/^\circ$	94.9150(10)	74.7925(16)
$\gamma/^\circ$	90	70.3241(17)
Volume/Å ³	32798.8(10)	21165.1(8)
Z	1	1
ρ_{calc}/cm^3	1.933	1.779
μ/mm^{-1}	20.326	19.441
F(000)	18508.0	10944.0
Radiation/Å	Cu K α ($\lambda = 1.54184$)	Cu K α ($\lambda = 1.54184$)
Reflections collected	218186	201709
Independent reflections	57831 [$R_{int} = 0.1043$, $R_{sigma} = 0.0811$]	74374 [$R_{int} = 0.0802$, $R_{sigma} = 0.0750$]
Data/parameters	57831/3616	74374/4300
Goodness-of-fit on F^2	1.271	1.067
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.1265$, $wR_2 = 0.3384$	$R_1 = 0.0846$, $wR_2 = 0.2504$
Final R indexes [all data]	$R_1 = 0.1717$, $wR_2 = 0.3781$	$R_1 = 0.1340$, $wR_2 = 0.2966$
Largest diff. peak/hole/eÅ ⁻³	2.63/-3.28	2.41/-2.28

Table S2: The formulae of the key species detected in positive-ion mode ESI-MS**of Ag₃₇ dissolved in MeOH/CH₂Cl₂.**

Peak	Species	Exp. <i>m/z</i>	Sim. <i>m/z</i>
1a	[NaCl ₇ @Ag ₃₆ (PTC4A) ₅ (<i>i</i> PrS) ₈] ²⁺	4370.551	4370.499
1b	[NaCl ₇ @Ag ₃₇ (PTC4A) ₅ (<i>i</i> PrS) ₆ (H ₂ O)(OH) ₃] ²⁺	4383.535	4383.434
1c	[NaCl ₆ @Ag ₃₆ (PTC4A) ₅ (<i>i</i> PrS) ₉ (H ₂ O)] ²⁺	4398.522	4398.527
1d	[NaCl ₇ @Ag ₃₇ (PTC4A) ₅ (<i>i</i> PrS) ₇ (H ₂ O)(OH) ₂] ²⁺	4412.498	4412.446
1e	[NaCl ₇ @Ag ₃₆ (PTC4A) ₅ (<i>i</i> PrS) ₈ (DMF)(CH ₃ CN)] ²⁺	4427.485	4427.539
1f	[NaCl ₇ @Ag ₃₇ (PTC4A) ₅ (<i>i</i> PrS) ₈ (H ₂ O)(OH)] ²⁺	4441.486	4441.458
1g	[NaCl ₆ @Ag ₃₆ (PTC4A) ₅ (<i>i</i> PrS) ₉ (H ₂ O)(DMF)(CH ₃ CN)] ²⁺	4455.460	4455.566
1h	[NaCl ₇ @Ag ₃₇ (PTC4A) ₅ (<i>i</i> PrS) ₉ (H ₂ O)] ²⁺	4470.961	4470.970

Table S3: The formulae of the key species detected in negative-ion mode ESI-MS

of Ag46 dissolved in MeOH/CH₂Cl₂.

Peak	Species	Exp. <i>m/z</i>	Sim. <i>m/z</i>
2a	[Cl ₆ @Ag ₄₄ (PTC4A) ₆ (ⁱ PrS) ₁₅ Cl] ²⁻	5451.8405	5451.7616
2b	[(CrO ₄)Cl ₆ @Ag ₄₄ (PTC4A) ₆ (ⁱ PrS) ₁₃ Cl(CH ₃ OH) ₂] ²⁻	5466.8209	5466.7212
2c	[Cl ₆ @Ag ₄₄ (PTC4A) ₆ (ⁱ PrS) ₁₆ (H ₂ O)] ²⁻	5480.8020	5480.7961

Table S4: The structure and dimension of dye molecules used in the dye-absorption experiments and the H₄PTC4A ligand.

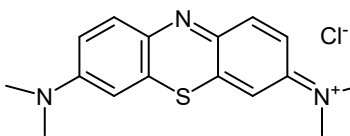
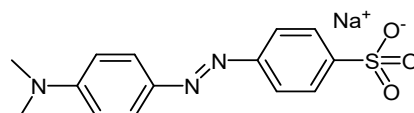
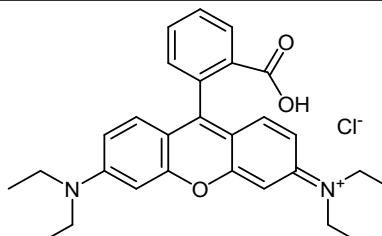
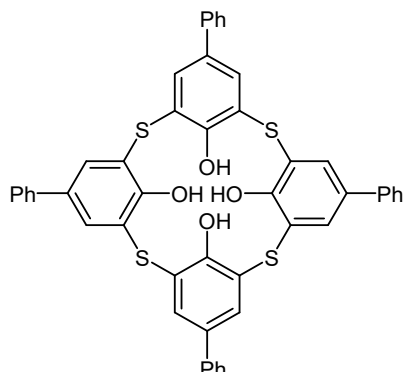
Dyes	Dyes structure	x (Å)	y (Å)	z (Å)
MB		4.00	7.93	16.34
MO		5.31	7.25	17.39
RhB		5.6	11.8	15.9
H₄PTC4A		7.4	9.9	14.7

Table S5: Various noncovalent interactions between Ag46 and dyes.

Dyes	Noncovalent interactions (Å)	
	$\pi \cdots \pi$	C-H $\cdots\pi$
MB	3.13, 3.79, 3.82	
RhB	3.33, 3.66, 4.00	3.04, 3.84

Table S6: Selected bond distances (Å) and bond angles (°) for Ag37 and Ag46.

Ag37			
Ag1—Ag16	3.333(3)	Ag16—S1	2.444(4)
Ag1—Ag24	3.303(3)	Ag16—S15	2.611(5)
Ag1—Ag30	3.315(3)	Ag16—O8	2.319(12)
Ag1—Ag31	3.278(3)	Ag16—O14	2.320(13)
Ag1—O3	2.545(14)	Ag17—Ag25	3.300(4)
Ag1—O8	2.312(13)	Ag17—O5	2.381(15)
Ag1—O14	2.505(13)	Ag17—O6	2.355(17)
Ag1—O19	2.23(1)	Ag17—O20	2.336(13)
Ag1—N2	2.32(2)	Ag17—O22	2.405(14)
Ag2—Ag6	3.116(6)	Ag17—O23	2.391(14)
Ag2—Ag30	2.948(3)	Ag18—Ag24	2.764(1)
Ag2—Cl3	2.795(6)	Ag18—S4	2.449(5)
Ag2—Cl8	2.673(5)	Ag18—S19	2.549(5)
Ag2—S20	2.404(5)	Ag18—O10	2.304(14)
Ag2—S22	2.425(5)	Ag18—O12	2.469(12)
Ag3—Ag5	3.220(13)	Ag19—Ag21	2.989(2)
Ag3—Ag7	3.084(3)	Ag19—Ag29	3.256(3)
Ag3—Ag25	3.227(3)	Ag19—S10	2.564(4)
Ag3—Ag37	3.372(3)	Ag19—S12	2.452(5)
Ag3—Cl6	2.664(5)	Ag19—O2	2.450(12)
Ag3—S12	2.430(5)	Ag19—O13	2.315(12)
Ag3—S17	2.356(6)	Ag20—S11	2.572(5)
Ag4—Ag18	2.964(3)	Ag20—S14	2.495(5)
Ag4—Ag20	3.083(3)	Ag20—O12	2.501(13)
Ag4—S4	2.453(4)	Ag20—O24	2.316(16)
Ag4—S14	2.527(4)	Ag21—Ag34	3.245(2)
Ag4—N5	2.43(3)	Ag21—Cl4	2.790(5)
Ag5—Ag35	3.276(12)	Ag21—S12	2.479(4)
Ag5—Ag37	3.320(11)	Ag21—S28	2.440(4)
Ag5—Cl1	2.541(12)	Ag22—Ag24	3.192(2)
Ag5—Cl3	2.586(11)	Ag22—Cl1	2.776(4)
Ag5—Cl6	2.621(12)	Ag22—Cl8	2.747(5)
Ag5—Cl11	2.591(10)	Ag22—S1	2.463(4)
Ag6—Ag22	3.225(5)	Ag22—S4	2.442(4)
Ag6—Ag27	3.256(5)	Ag23—Ag25	3.060(2)
Ag6—Ag34	3.371(5)	Ag23—Ag37	3.026(2)
Ag6—Cl1	2.766(7)	Ag23—S17	2.399(5)
Ag6—Cl3	2.575(8)	Ag23—S29	2.526(7)
Ag6—Cl8	2.610(7)	Ag23—O24	2.275(15)

Ag23—O17	2.634(5)	Ag37—S20	2.439(4)
Ag6—Cl10	2.559(7)	Ag24—S4	2.545(4)
Ag7—Ag17	3.300(3)	Ag24—S24	2.629(5)
Ag7—Ag19	2.8654(19)	Ag24—O14	2.389(12)
Ag7—S12	2.502(4)	Ag24—O19	2.339(13)
Ag7—S16	2.580(4)	Ag25—S13	2.564(5)
Ag7—O20	2.369(13)	Ag25—S17	2.426(4)
Ag7—O22	2.396(13)	Ag25—O6	2.380(15)
Ag8—Ag18	3.241(3)	Ag25—O22	2.459(13)
Ag8—Ag20	3.327(3)	Ag26—Ag28	3.313(3)
Ag8—Ag23	3.317(3)	Ag26—Ag32	3.287(3)
Ag8—Ag33	3.305(3)	Ag26—O4	2.391(13)
Ag8—Cl11	2.904(7)	Ag26—O15	2.447(13)
Ag8—O1	2.52(3)	Ag26—O16	2.36(2)
Ag8—O10	2.512(13)	Ag26—O18	2.357(13)
Ag8—O12	2.255(15)	Ag26—O21	2.416(14)
Ag8—O17	2.240(14)	Ag27—Ag28	3.073(2)
Ag8—O24	2.586(14)	Ag27—Cl10	2.681(5)
Ag9—Ag27	3.205(2)	Ag27—S1	2.425(4)
Ag9—Ag36	3.098(2)	Ag27—S6	2.422(4)
Ag9—Cl1	2.854(5)	Ag28—S6	2.444(4)
Ag9—Cl4	2.664(5)	Ag28—S27	2.549(6)
Ag9—S6	2.482(5)	Ag28—O15	2.343(13)
Ag9—S8	2.472(4)	Ag28—O16	2.500(16)
Ag10—Ag16	2.8083(18)	Ag29—Ag36	3.294(3)
Ag10—Ag26	3.285(3)	Ag29—O2	2.281(12)
Ag10—Ag27	3.1894(18)	Ag29—O7	2.255(13)
Ag10—S1	2.519(4)	Ag29—O11	2.236(15)
Ag10—S3	2.582(5)	Ag29—O13	2.475(13)
Ag10—O4	2.379(13)	Ag30—Ag33	2.926(2)
Ag10—O16	2.400(17)	Ag30—S20	2.427(4)
Ag11—Ag17	3.236(3)	Ag30—S21	2.581(5)
Ag11—Ag20	2.8574(17)	Ag30—O3	2.369(15)
Ag11—S2	2.603(4)	Ag30—O19	2.371(13)
Ag11—S14	2.473(4)	Ag31—Ag32	2.805(2)
Ag11—O6	2.300(16)	Ag31—S7	2.612(5)
Ag11—O23	2.393(13)	Ag31—S22	2.516(4)
Ag12—Ag14	2.8741(16)	Ag31—O3	2.338(18)
Ag12—Ag29	3.370(3)	Ag31—O8	2.393(13)
Ag12—S18	2.630(5)	Ag32—Ag34	2.955(2)
Ag12—S28	2.461(5)	Ag32—S5	2.556(5)
Ag12—O2	2.451(10)	Ag32—S22	2.439(5)
Ag12—O9	2.324(14)	Ag32—O4	2.347(14)

Ag13—Ag15	2.7939(19)	Ag32—O18	2.345(12)
Ag13—Ag17	3.264(4)	Ag33—Ag37	3.134(2)
Ag13—Ag35	2.9670(17)	Ag33—S20	2.461(5)
Ag13—S8	2.459(4)	Ag33—S25	2.547(6)
Ag13—S26	2.581(4)	Ag33—O10	2.328(14)
Ag13—O20	2.409(12)	Ag33—O17	2.576(14)
Ag13—O23	2.333(13)	Ag34—Cl10	2.904(5)
Ag14—Ag26	3.258(3)	Ag34—S22	2.416(5)
Ag14—Ag34	3.366(2)	Ag34—S28	2.408(5)
Ag14—S9	2.570(5)	Ag35—Cl6	2.924(5)
Ag14—S28	2.489(5)	Ag35—S8	2.486(5)
Ag14—O15	2.330(15)	Ag35—S14	2.462(5)
Ag14—O18	2.467(11)	Ag36—S6	2.444(4)
Ag15—Ag29	3.363(3)	Ag36—S23	2.576(6)
Ag15—S8	2.522(4)	Ag36—O7	2.506(12)
Ag15—S30	2.626(5)	Ag36—O9	2.344(12)
Ag15—O7	2.435(13)	Ag37—Cl11	2.626(6)
Ag15—O13	2.358(11)	Ag37—S17	2.454(4)
Ag16—Ag22	3.1739(18)		
O8—Ag1—O3	88.6(5)	O20—Ag17—O6	164.3(4)
O8—Ag1—O14	84.6(4)	O20—Ag17—O22	87.4(5)
O8—Ag1—N2	96.2(7)	O20—Ag17—O23	89.2(5)
O14—Ag1—O3	153.5(4)	O23—Ag17—O22	162.2(4)
O19—Ag1—O3	88.4(5)	S4—Ag18—S19	128.17(16)
O19—Ag1—O8	155.1(4)	S4—Ag18—O12	119.5(4)
O19—Ag1—O14	87.2(5)	O10—Ag18—S4	142.5(4)
O19—Ag1—N2	108.3(7)	O10—Ag18—S19	79.4(4)
N2—Ag1—O3	105.8(5)	O10—Ag18—O12	89.3(5)
N2—Ag1—O14	100.4(5)	O12—Ag18—S19	75.8(3)
Cl8—Ag2—Cl3	96.20(19)	S12—Ag19—S10	123.54(15)
S20—Ag2—Cl3	101.63(19)	O2—Ag19—S10	75.1(3)
S20—Ag2—Cl8	105.17(18)	O2—Ag19—S12	132.4(3)
S20—Ag2—S22	142.30(19)	O13—Ag19—S10	78.2(3)
S22—Ag2—Cl3	104.36(18)	O13—Ag19—S12	134.5(3)
S22—Ag2—Cl8	98.68(18)	O13—Ag19—O2	89.4(4)
S12—Ag3—Cl6	107.77(18)	S14—Ag20—S11	125.54(17)
S17—Ag3—Cl6	104.06(19)	S14—Ag20—O12	116.6(4)
S17—Ag3—S12	143.78(19)	O12—Ag20—S11	74.0(3)
S4—Ag4—S14	142.5(2)	O24—Ag20—S11	77.4(4)
N5—Ag4—S4	109.2(6)	O24—Ag20—S14	149.6(4)
N5—Ag4—S14	103.2(7)	O24—Ag20—O12	87.1(5)
Cl1—Ag5—Cl3	95.6(3)	S12—Ag21—Cl4	101.43(16)
Cl1—Ag5—Cl6	110.4(5)	S28—Ag21—Cl4	94.89(17)

Cl1—Ag5—Cl11	117.8(5)	S28—Ag21—S12	153.43(16)
Cl3—Ag5—Cl6	108.3(4)	Cl8—Ag22—Cl1	98.85(16)
Cl3—Ag5—Cl11	116.7(5)	S1—Ag22—Cl8	98.32(16)
Cl11—Ag5—Cl6	107.5(3)	S4—Ag22—Cl1	103.43(13)
Cl3—Ag6—Cl1	90.6(2)	S4—Ag22—Cl8	105.26(17)
Cl3—Ag6—Cl8	103.5(3)	S1—Ag22—Cl1	98.14(15)
S20—Ag37—S17	143.62(18)	S4—Ag22—S1	144.87(15)
Cl8—Ag6—Cl1	102.6(2)	S17—Ag23—S29	132.7(2)
Cl10—Ag6—Cl1	114.5(2)	O24—Ag23—S17	144.1(4)
Cl10—Ag6—Cl3	117.3(2)	O24—Ag23—S29	79.6(4)
Cl10—Ag6—Cl8	122.9(3)	S4—Ag24—S24	116.29(15)
S12—Ag7—S16	125.30(15)	O14—Ag24—S4	107.6(3)
O20—Ag7—S12	153.1(3)	O14—Ag24—S24	76.7(3)
O20—Ag7—S16	75.1(3)	O19—Ag24—S4	162.9(3)
O20—Ag7—O22	86.8(4)	O19—Ag24—S24	74.3(3)
O22—Ag7—S12	113.4(3)	O19—Ag24—O14	87.6(4)
O22—Ag7—S16	76.2(3)	S17—Ag25—S13	136.7(2)
O1—Ag8—Cl11	169.2(11)	S17—Ag25—O22	113.0(3)
O1—Ag8—O24	100.9(12)	O6—Ag25—S13	77.3(4)
O10—Ag8—Cl11	84.0(3)	O6—Ag25—S17	141.4(3)
O10—Ag8—O1	91.3(12)	O6—Ag25—O22	88.9(5)
O10—Ag8—O24	167.0(5)	O22—Ag25—S13	76.9(3)
O12—Ag8—Cl11	82.0(4)	O4—Ag26—O15	164.3(4)
O12—Ag8—O1	88.3(12)	O4—Ag26—O21	96.4(5)
O12—Ag8—O10	89.3(4)	O16—Ag26—O4	88.5(5)
O12—Ag8—O24	86.4(5)	O16—Ag26—O15	91.0(5)
O17—Ag8—Cl11	89.0(4)	O16—Ag26—O21	100.9(6)
O17—Ag8—O1	100.8(12)	O18—Ag26—O4	86.5(5)
O17—Ag8—O10	90.9(5)	O18—Ag26—O15	89.7(5)
O17—Ag8—O12	170.9(6)	O18—Ag26—O16	164.1(5)
O17—Ag8—O24	91.5(5)	O18—Ag26—O21	94.7(5)
O24—Ag8—Cl11	83.2(3)	O21—Ag26—O15	99.0(6)
Cl4—Ag9—Cl1	103.25(17)	S1—Ag27—Cl10	104.81(16)
S6—Ag9—Cl1	114.26(14)	S6—Ag27—Cl10	103.26(16)
S6—Ag9—Cl4	102.67(16)	S6—Ag27—S1	150.60(15)
S8—Ag9—Cl1	89.63(15)	S6—Ag28—S27	137.33(17)
S8—Ag9—Cl4	102.91(16)	S6—Ag28—O16	118.1(4)
S8—Ag9—S6	139.43(17)	O15—Ag28—S6	136.5(4)
S1—Ag10—S3	126.09(15)	O15—Ag28—S27	78.8(4)
O4—Ag10—S1	154.1(4)	O15—Ag28—O16	90.1(5)
O4—Ag10—S3	76.2(3)	O16—Ag28—S27	75.1(4)
O4—Ag10—O16	87.9(6)	O2—Ag29—O13	89.6(4)
O16—Ag10—S1	108.4(4)	O7—Ag29—O2	161.8(5)

O16—Ag10—S3	77.7(4)	O7—Ag29—O13	87.1(4)
S14—Ag11—S2	125.55(16)	O11—Ag29—O2	98.4(6)
O6—Ag11—S2	76.4(3)	O11—Ag29—O7	99.8(6)
O6—Ag11—S14	156.3(4)	O11—Ag29—O13	100.6(5)
O6—Ag11—O23	89.0(5)	S20—Ag30—S21	128.48(18)
O23—Ag11—S2	76.1(3)	O3—Ag30—S20	130.9(4)
O23—Ag11—S14	104.2(3)	O3—Ag30—S21	76.7(4)
S28—Ag12—S18	130.38(16)	O3—Ag30—O19	89.5(5)
O2—Ag12—S18	74.4(3)	O19—Ag30—S20	132.8(3)
O2—Ag12—S28	107.1(3)	O19—Ag30—S21	77.3(3)
O9—Ag12—S18	77.0(3)	S22—Ag31—S7	129.47(17)
O9—Ag12—S28	150.2(3)	O3—Ag31—S7	76.3(3)
O9—Ag12—O2	90.3(4)	O3—Ag31—S22	99.7(4)
S8—Ag13—S26	125.02(17)	O3—Ag31—O8	91.7(5)
O20—Ag13—S8	131.7(3)	O8—Ag31—S7	74.2(3)
O20—Ag13—S26	77.0(3)	O8—Ag31—S22	155.5(3)
O23—Ag13—S8	134.1(3)	S22—Ag32—S5	128.55(17)
O23—Ag13—S26	78.3(3)	O4—Ag32—S5	78.3(3)
O23—Ag13—O20	88.9(4)	O4—Ag32—S22	134.9(3)
S28—Ag14—S9	128.98(16)	O18—Ag32—S5	77.1(3)
O15—Ag14—S9	77.5(3)	O18—Ag32—S22	129.3(3)
O15—Ag14—S28	149.5(3)	O18—Ag32—O4	87.8(5)
O15—Ag14—O18	89.9(4)	S20—Ag33—S25	130.92(19)
O18—Ag14—S9	75.5(3)	S20—Ag33—O17	107.2(3)
O18—Ag14—S28	109.8(3)	S25—Ag33—O17	74.5(4)
S8—Ag15—S30	130.97(16)	O10—Ag33—S20	150.2(4)
O7—Ag15—S8	108.3(3)	O10—Ag33—S25	77.5(4)
O7—Ag15—S30	75.4(3)	O10—Ag33—O17	87.4(4)
O13—Ag15—S8	151.4(3)	S22—Ag34—Cl10	99.74(16)
O13—Ag15—S30	76.0(3)	S28—Ag34—Cl10	93.87(17)
O13—Ag15—O7	85.8(4)	S28—Ag34—S22	164.46(17)
S1—Ag16—S15	128.18(17)	S8—Ag35—Cl6	98.02(16)
O8—Ag16—S1	141.8(3)	S14—Ag35—Cl6	91.43(16)
O8—Ag16—S15	76.7(3)	S14—Ag35—S8	158.87(15)
O8—Ag16—O14	88.7(4)	S6—Ag36—S23	127.54(17)
O14—Ag16—S1	122.8(3)	S6—Ag36—O7	129.5(3)
O14—Ag16—S15	75.3(3)	O7—Ag36—S23	72.6(3)
O5—Ag17—O22	98.6(5)	O9—Ag36—S6	134.7(3)
O5—Ag17—O23	99.2(5)	O9—Ag36—S23	77.6(4)
O6—Ag17—O5	96.7(5)	O9—Ag36—O7	91.5(4)
O6—Ag17—O22	90.8(5)	S17—Ag37—Cl11	108.44(17)
O6—Ag17—O23	87.8(5)	S20—Ag37—Cl11	107.94(16)
O20—Ag17—O5	99.0(5)	S20—Ag37—S17	143.62(18)

Ag46			
Ag1—Ag2	2.89(2)	Ag22—S20	2.485(3)
Ag1—Ag41	2.95(3)	Ag22—O30	2.388(11)
Ag1—Ag43	3.05(3)	Ag22—O32	2.276(9)
Ag1—Cl2	2.32(3)	Ag23—Ag42	3.2935(18)
Ag1—O2	2.18(3)	Ag23—Ag44	3.315(2)
Ag2—Ag29	2.981(6)	Ag23—Ag45	2.820(2)
Ag2—Ag38	3.021(5)	Ag23—S15	2.583(4)
Ag2—Cl3	2.407(8)	Ag23—S21	2.472(3)
Ag3—Ag10	3.151(6)	Ag23—O10	2.408(12)
Ag3—Ag27	3.313(7)	Ag23—O14	2.356(9)
Ag3—Ag42	3.241(6)	Ag24—Ag41	3.0560(17)
Ag3—Cl1	2.730(9)	Ag24—S3	2.596(4)
Ag3—Cl4	2.690(9)	Ag24—S18	2.470(3)
Ag3—O4	2.14(2)	Ag24—O12	2.429(10)
Ag4—Ag12	3.052(9)	Ag24—O27	2.306(8)
Ag4—Ag35	2.953(10)	Ag25—Ag37	3.0415(17)
Ag4—Cl5	2.306(13)	Ag25—Cl6	2.858(5)
Ag5—Ag15	3.231(5)	Ag25—S8	2.412(3)
Ag5—Ag22	3.228(5)	Ag25—S24	2.414(3)
Ag5—Ag28	3.233(5)	Ag25—O2	2.51(2)
Ag5—Ag33	3.198(6)	Ag26—Ag28	2.8447(16)
Ag5—O28	2.115(11)	Ag26—Ag29	3.0672(19)
Ag5—O30	2.136(10)	Ag26—S6	2.484(3)
Ag6—Ag19	3.254(5)	Ag26—S29	2.621(4)
Ag6—Ag26	3.187(5)	Ag26—O16	2.349(12)
Ag6—Ag36	3.204(6)	Ag26—O19	2.408(10)
Ag6—O17	2.025(12)	Ag27—Ag33	3.3414(15)
Ag6—O19	2.054(12)	Ag27—Cl1	2.811(4)
Ag7—Ag17	3.163(3)	Ag27—S20	2.430(4)
Ag7—Ag24	3.140(4)	Ag27—S28	2.438(4)
Ag7—Ag30	3.055(4)	Ag28—S6	2.501(3)
Ag7—Ag39	3.146(4)	Ag28—S19	2.625(4)
Ag7—Cl2	2.882(7)	Ag28—O26	2.362(9)
Ag7—O9	2.104(11)	Ag28—O30	2.376(11)
Ag7—O12	2.040(12)	Ag29—Cl3	2.841(5)
Ag7—O22	2.525(12)	Ag29—S6	2.424(3)
Ag7—O27	2.594(13)	Ag29—S18	2.411(3)
Ag8—Ag13	3.377(10)	Ag30—Ag36	2.8298(18)
Ag8—Ag31	3.325(10)	Ag30—S14	2.492(4)
Ag8—Ag34	3.078(12)	Ag30—S26	2.610(4)
Ag8—Ag37	2.961(11)	Ag30—O12	2.362(11)
Ag8—O13	1.944(16)	Ag30—O22	2.398(10)

Ag8—O23	1.981(17)	Ag31—Ag39	2.8295(17)
Ag9—Ag15	2.8069(14)	Ag31—S22	2.444(4)
Ag9—Ag44	3.243(2)	Ag31—S23	2.624(4)
Ag9—S4	2.487(3)	Ag31—O21	2.276(13)
Ag9—S16	2.571(3)	Ag31—O23	2.476(11)
Ag9—O20	2.438(9)	Ag32—Ag34	3.0004(18)
Ag9—O25	2.373(9)	Ag32—Cl6	2.808(5)
Ag10—Ag15	3.0503(13)	Ag32—S5	2.418(4)
Ag10—Cl1	2.810(4)	Ag32—S22	2.408(3)
Ag10—S4	2.445(3)	Ag32—O5	2.53(3)
Ag10—S6	2.440(3)	Ag33—S27	2.609(4)
Ag10—O4	2.52(2)	Ag33—S28	2.499(4)
Ag11—Ag14	3.0247(14)	Ag33—O28	2.369(11)
Ag11—Ag20	2.7947(15)	Ag33—O32	2.357(11)
Ag11—Ag44	3.212(2)	Ag34—Ag40	2.8520(19)
Ag11—S1	2.470(3)	Ag34—S5	2.494(4)
Ag11—S12	2.583(3)	Ag34—S7	2.611(4)
Ag11—O14	2.345(11)	Ag34—O15	2.355(11)
Ag11—O20	2.346(9)	Ag34—O23	2.388(12)
Ag12—Ag16	3.0380(15)	Ag35—Ag45	3.157(2)
Ag12—Cl5	2.821(5)	Ag35—Cl5	2.798(5)
Ag12—S1	2.434(3)	Ag35—S5	2.400(4)
Ag12—S8	2.440(3)	Ag35—S21	2.424(4)
Ag12—O3	2.56(2)	Ag36—Ag38	3.0056(17)
Ag13—Ag16	2.8471(13)	Ag36—S14	2.467(4)
Ag13—S8	2.500(3)	Ag36—S36	2.610(4)
Ag13—S10	2.651(4)	Ag36—O17	2.392(10)
Ag13—O13	2.467(9)	Ag36—O24	2.333(10)
Ag13—O15	2.271(10)	Ag37—Cl6	2.917(5)
Ag14—Cl4	2.832(4)	Ag37—S2	2.663(4)
Ag14—S1	2.434(3)	Ag37—S24	2.477(4)
Ag14—S4	2.438(3)	Ag37—O13	2.378(9)
Ag15—S4	2.492(3)	Ag37—O21	2.320(11)
Ag15—S30	2.626(4)	Ag38—Cl3	2.825(5)
Ag15—O26	2.312(10)	Ag38—S14	2.397(3)
Ag15—O28	2.386(10)	Ag38—S20	2.403(3)
Ag16—Ag46	3.320(2)	Ag39—Ag43	3.0581(18)
Ag16—S8	2.464(3)	Ag39—S22	2.456(4)
Ag16—S13	2.586(4)	Ag39—S31	2.605(4)
Ag16—O11	2.326(9)	Ag39—O9	2.409(11)
Ag16—O29	2.370(11)	Ag39—O22	2.310(10)
Ag17—Ag37	2.8487(16)	Ag40—Ag46	3.360(2)
Ag17—S9	2.607(4)	Ag40—S5	2.481(4)

Ag17—S24	2.510(3)	Ag40—S17	2.587(5)
Ag17—O9	2.404(10)	Ag40—O29	2.381(12)
Ag17—O27	2.375(9)	Ag40—O31	2.392(17)
Ag18—Ag24	2.8268(16)	Ag41—Cl2	2.866(5)
Ag18—S18	2.457(3)	Ag41—S18	2.422(4)
Ag18—S34	2.632(4)	Ag41—S24	2.401(4)
Ag18—O19	2.461(9)	Ag42—Cl4	2.795(4)
Ag18—O24	2.292(10)	Ag42—S21	2.404(4)
Ag19—Ag22	2.7756(15)	Ag42—S28	2.414(4)
Ag19—S20	2.476(4)	Ag43—Cl2	2.779(6)
Ag19—S25	2.640(5)	Ag43—S14	2.406(4)
Ag19—O16	2.276(12)	Ag43—S22	2.420(4)
Ag19—O17	2.415(9)	Ag44—O10	2.344(12)
Ag20—Ag46	3.298(2)	Ag44—O14	2.429(11)
Ag20—S1	2.537(3)	Ag44—O20	2.368(9)
Ag20—S32	2.587(3)	Ag44—O25	2.499(10)
Ag20—O11	2.397(10)	Ag44—N5	2.309(17)
Ag20—O18	2.402(12)	Ag45—Ag46	3.288(3)
Ag21—Ag33	2.7747(18)	Ag45—S21	2.457(4)
Ag21—Ag42	3.1475(17)	Ag45—S35	2.574(6)
Ag21—Ag44	3.2206(19)	Ag45—O18	2.412(13)
Ag21—S28	2.475(3)	Ag45—O31	2.362(15)
Ag21—S33	2.553(4)	Ag46—O11	2.505(11)
Ag21—O10	2.396(12)	Ag46—O18	2.312(12)
Ag21—O25	2.374(10)	Ag46—O29	2.270(11)
Ag22—Ag27	3.0704(18)	Ag46—O31	2.438(15)
Ag22—S11	2.628(4)	Ag46—N6	2.43(2)
O2—Ag1—Cl2	139.0(15)	O16—Ag26—S6	130.0(3)
Cl4—Ag3—Cl1	116.1(2)	O16—Ag26—S29	76.3(3)
O4—Ag3—Cl1	96.9(7)	O16—Ag26—O19	90.8(3)
O4—Ag3—Cl4	121.8(6)	O19—Ag26—S6	137.9(3)
O28—Ag5—O30	162.4(5)	O19—Ag26—S29	73.8(2)
O17—Ag6—O19	161.0(5)	S20—Ag27—Cl1	99.60(12)
O9—Ag7—Cl2	87.1(3)	S20—Ag27—S28	153.96(13)
O9—Ag7—O22	89.3(4)	S28—Ag27—Cl1	95.64(12)
O9—Ag7—O27	88.2(4)	S6—Ag28—S19	126.95(13)
O12—Ag7—Cl2	91.5(3)	O26—Ag28—S6	105.0(3)
O12—Ag7—O9	178.2(5)	O26—Ag28—S19	75.3(2)
O12—Ag7—O22	91.9(4)	O26—Ag28—O30	91.1(3)
O12—Ag7—O27	90.4(4)	O30—Ag28—S6	156.4(3)
O22—Ag7—Cl2	87.1(3)	O30—Ag28—S19	73.4(3)
O22—Ag7—O27	168.8(4)	S6—Ag29—Cl3	97.38(14)
O27—Ag7—Cl2	81.9(3)	S18—Ag29—Cl3	97.19(13)

O13—Ag8—O23	168.4(8)	S18—Ag29—S6	148.48(13)
S4—Ag9—S16	134.42(12)	S14—Ag30—S26	126.99(13)
O20—Ag9—S4	107.8(2)	O12—Ag30—S14	157.7(3)
O20—Ag9—S16	75.7(2)	O12—Ag30—S26	74.5(3)
O25—Ag9—S4	145.5(2)	O12—Ag30—O22	87.7(4)
O25—Ag9—S16	76.9(2)	O22—Ag30—S14	102.6(3)
O25—Ag9—O20	92.3(3)	O22—Ag30—S26	75.7(3)
S4—Ag10—Cl1	102.86(11)	S22—Ag31—S23	126.44(15)
S4—Ag10—O4	104.3(5)	S22—Ag31—O23	119.6(3)
S6—Ag10—Cl1	93.32(12)	O21—Ag31—S22	149.2(3)
S6—Ag10—S4	149.92(12)	O21—Ag31—S23	77.7(3)
S6—Ag10—O4	101.8(5)	O21—Ag31—O23	83.3(4)
O4—Ag10—Cl1	86.7(5)	O23—Ag31—S23	72.8(3)
S1—Ag11—S12	125.90(11)	S5—Ag32—Cl6	93.09(15)
O14—Ag11—S1	133.1(2)	S5—Ag32—O5	112.3(6)
O14—Ag11—S12	76.9(2)	S22—Ag32—Cl6	102.81(14)
O14—Ag11—O20	90.9(3)	S22—Ag32—S5	150.99(13)
O20—Ag11—S1	131.2(2)	S22—Ag32—O5	92.8(6)
O20—Ag11—S12	76.8(2)	O5—Ag32—Cl6	87.2(6)
S1—Ag12—Cl5	93.46(14)	S28—Ag33—S27	123.79(14)
S1—Ag12—S8	151.84(11)	O28—Ag33—S27	74.1(2)
S1—Ag12—O3	87.2(5)	O28—Ag33—S28	156.0(3)
S8—Ag12—Cl5	102.15(16)	O32—Ag33—S27	77.0(2)
S8—Ag12—O3	102.2(5)	O32—Ag33—S28	108.3(3)
O3—Ag12—Cl5	125.1(5)	O32—Ag33—O28	90.5(4)
S8—Ag13—S10	124.29(12)	S5—Ag34—S7	120.21(14)
O13—Ag13—S8	119.2(2)	O15—Ag34—S5	123.0(2)
O13—Ag13—S10	71.6(2)	O15—Ag34—S7	77.2(3)
O15—Ag13—S8	151.6(3)	O15—Ag34—O23	93.4(4)
O15—Ag13—S10	77.1(3)	O23—Ag34—S5	142.3(3)
O15—Ag13—O13	83.5(3)	O23—Ag34—S7	73.7(3)
S1—Ag14—Cl4	101.48(14)	S5—Ag35—Cl5	101.63(17)
S1—Ag14—S4	157.49(10)	S5—Ag35—S21	150.16(15)
S4—Ag14—Cl4	91.03(13)	S21—Ag35—Cl5	95.72(15)
S4—Ag15—S30	123.86(11)	S14—Ag36—S36	121.63(12)
O26—Ag15—S4	124.2(3)	O17—Ag36—S14	141.2(3)
O26—Ag15—S30	77.1(2)	O17—Ag36—S36	74.5(2)
O26—Ag15—O28	92.1(4)	O24—Ag36—S14	126.8(2)
O28—Ag15—S4	140.6(3)	O24—Ag36—S36	76.7(2)
O28—Ag15—S30	74.9(2)	O24—Ag36—O17	89.8(3)
S8—Ag16—S13	129.32(14)	S2—Ag37—Cl6	152.75(15)
O11—Ag16—S8	133.1(2)	S24—Ag37—Cl6	94.07(14)
O11—Ag16—S13	76.4(2)	S24—Ag37—S2	112.94(15)

O11—Ag16—O29	88.3(3)	O13—Ag37—Cl6	83.4(3)
O29—Ag16—S8	131.4(2)	O13—Ag37—S2	73.7(2)
O29—Ag16—S13	76.5(3)	O13—Ag37—S24	139.9(3)
S24—Ag17—S9	121.07(13)	O21—Ag37—Cl6	92.1(3)
O9—Ag17—S9	74.3(3)	O21—Ag37—S2	74.8(3)
O9—Ag17—S24	163.7(3)	O21—Ag37—S24	127.1(3)
O27—Ag17—S9	75.7(2)	O21—Ag37—O13	93.0(4)
O27—Ag17—S24	101.7(3)	S14—Ag38—Cl3	97.24(14)
O27—Ag17—O9	87.0(4)	S14—Ag38—S20	154.97(13)
S18—Ag18—S34	125.72(13)	S20—Ag38—Cl3	93.53(15)
S18—Ag18—O19	116.9(3)	S22—Ag39—S31	129.95(13)
O19—Ag18—S34	73.2(2)	O9—Ag39—S22	135.3(3)
O24—Ag18—S18	151.1(3)	O9—Ag39—S31	75.0(2)
O24—Ag18—S34	77.0(3)	O22—Ag39—S22	130.0(3)
O24—Ag18—O19	84.7(3)	O22—Ag39—S31	76.9(3)
S20—Ag19—S25	128.02(14)	O22—Ag39—O9	87.5(4)
O16—Ag19—S20	147.1(3)	S5—Ag40—S17	124.97(15)
O16—Ag19—S25	76.2(3)	O29—Ag40—S5	157.7(3)
O16—Ag19—O17	88.7(3)	O29—Ag40—S17	75.6(3)
O17—Ag19—S20	117.8(3)	O29—Ag40—O31	84.8(5)
O17—Ag19—S25	72.7(2)	O31—Ag40—S5	107.3(4)
S1—Ag20—S32	130.59(12)	O31—Ag40—S17	75.5(3)
O11—Ag20—S1	104.3(2)	S18—Ag41—Cl2	97.95(16)
O11—Ag20—S32	76.2(2)	S24—Ag41—Cl2	94.33(16)
O11—Ag20—O18	89.8(4)	S24—Ag41—S18	155.63(14)
O18—Ag20—S1	152.9(3)	S21—Ag42—Cl4	104.66(14)
O18—Ag20—S32	74.9(3)	S21—Ag42—S28	149.86(14)
S28—Ag21—S33	130.28(13)	S28—Ag42—Cl4	97.98(14)
O10—Ag21—S28	123.5(3)	S14—Ag43—Cl2	96.99(17)
O10—Ag21—S33	76.0(3)	S14—Ag43—S22	148.86(13)
O25—Ag21—S28	136.8(2)	S22—Ag43—Cl2	99.35(17)
O25—Ag21—S33	77.6(2)	O10—Ag44—O14	86.8(4)
O25—Ag21—O10	92.1(4)	O10—Ag44—O20	165.7(3)
S20—Ag22—S11	125.28(12)	O10—Ag44—O25	90.3(4)
O30—Ag22—S11	74.7(3)	O14—Ag44—O25	164.8(3)
O30—Ag22—S20	142.0(3)	O20—Ag44—O14	88.4(3)
O32—Ag22—S11	76.3(3)	O20—Ag44—O25	90.9(3)
O32—Ag22—S20	123.6(3)	N5—Ag44—O10	96.6(6)
O32—Ag22—O30	90.6(4)	N5—Ag44—O14	94.8(5)
S21—Ag23—S15	124.88(14)	N5—Ag44—O20	97.2(6)
O10—Ag23—S15	76.3(3)	N5—Ag44—O25	100.4(5)
O10—Ag23—S21	111.4(3)	S21—Ag45—S35	131.93(17)
O14—Ag23—S15	76.9(3)	O18—Ag45—S21	134.0(3)

O14—Ag23—S21	153.4(3)	O18—Ag45—S35	76.8(3)
O14—Ag23—O10	87.0(4)	O31—Ag45—S21	127.2(4)
S18—Ag24—S3	129.82(12)	O31—Ag45—S35	77.4(4)
O12—Ag24—S3	75.2(3)	O31—Ag45—O18	89.4(5)
O12—Ag24—S18	136.0(3)	O18—Ag46—O11	89.3(4)
O27—Ag24—S3	77.4(3)	O18—Ag46—O31	89.9(5)
O27—Ag24—S18	128.1(3)	O18—Ag46—N6	103.5(6)
O27—Ag24—O12	88.7(4)	O29—Ag46—O11	86.4(4)
S8—Ag25—Cl6	94.72(14)	O29—Ag46—O18	158.8(4)
S8—Ag25—S24	149.55(13)	O29—Ag46—O31	86.2(5)
S8—Ag25—O2	110.8(6)	O29—Ag46—N6	97.7(6)
S24—Ag25—Cl6	96.99(14)	O31—Ag46—O11	157.4(4)
S24—Ag25—O2	98.4(6)	N6—Ag46—O11	101.4(5)
O2—Ag25—Cl6	84.1(6)	N6—Ag46—O31	100.7(6)
S6—Ag26—S29	119.90(13)		

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