Electronic Supplementary Material (ESI) for Nanoscale
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Supporting Information

1. Characterizations of the AgISNPs and BNPs

For PXRD pattern of AgI SNPs (Fig. 1(b)), based on the first peak, the grain size of the AgI SNPs calculated from the Scherrer's equation[S1] ($D = 0.89\lambda/\beta\cos\theta$, where λ, β and θ are the wavelength of incident X-ray, FWHM of diffraction peak in radian and the diffraction angle, respectively.) is 1.0 nm.

The XPS (Fig S1) clearly show the Ag $3d_{3/2}$ and $3d_{5/2}$ peaks at 374nm and 368nm and the I $3d_{3/2}$ and $3d_{5/2}$ peaks at 631nm and 619 nm for AgI SNPs (2) and AgI BNPs (3), which confirm that Ag and I are in +1 and -1 valence compared with bulk AgI powders (1).

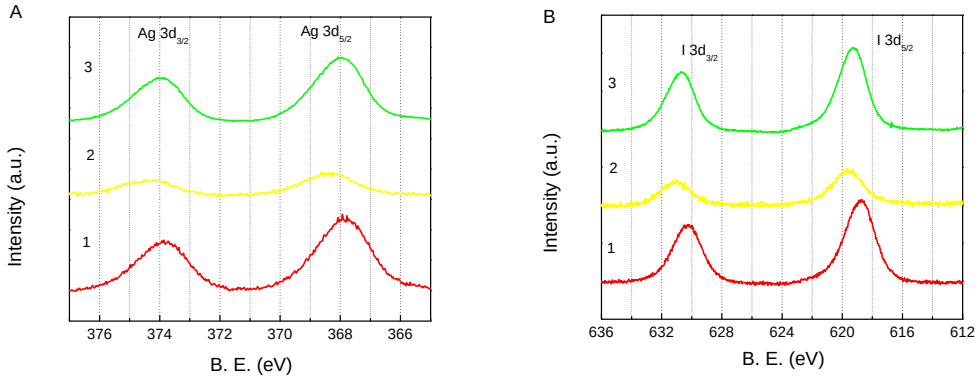

Fig. S1 XPS profiles of a) Ag 3d peaks and b) I 3d peaks of AgI Bulk (red), AgI SNPs (yellow) and AgI BNPs (green)

Reference

S1 B. E. Warren, *X-ray Diffraction*; Constable and Company Ltd. U.K., London, **1990**;

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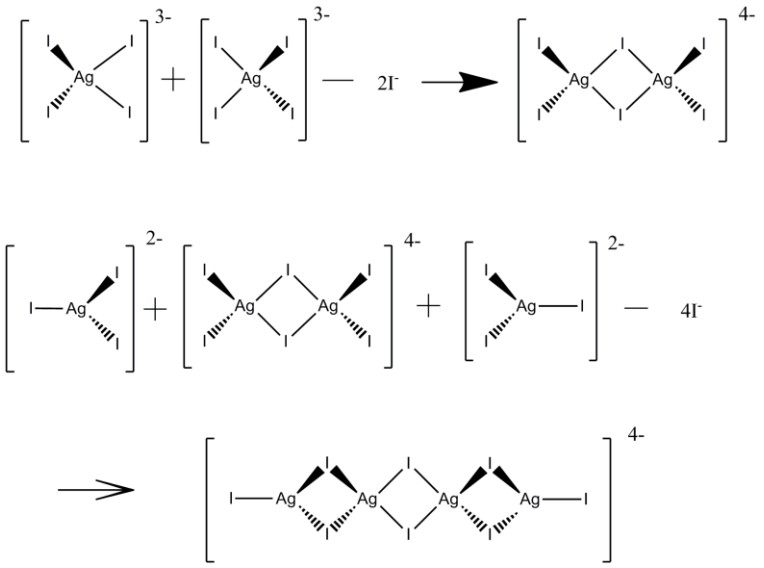
2. Growth processes



Scheme S2 Formation process of $[Ag_4I_8]^{4-}$ in **2**

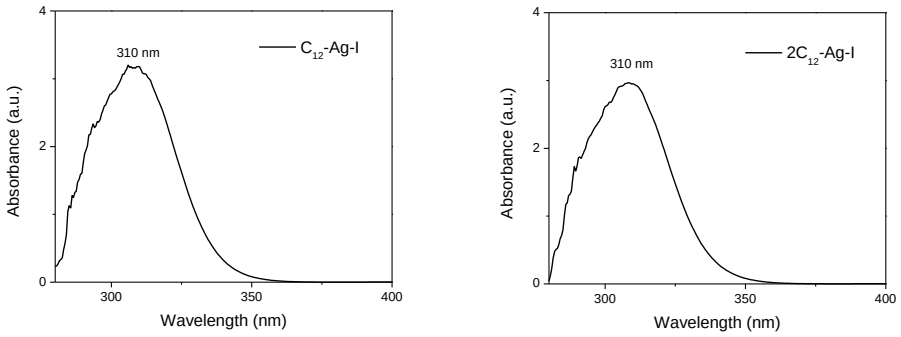
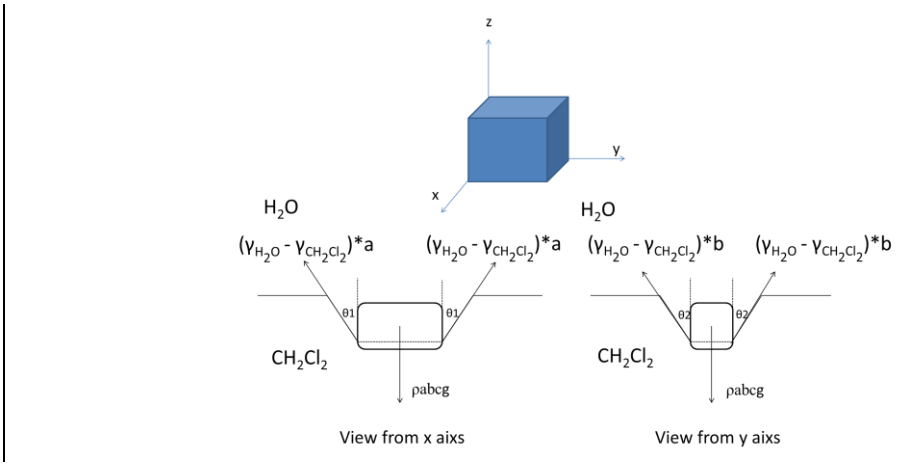


Fig S2 UV-Vis spectra of the CH_2Cl_2 phase after layering water phase and the CH_2Cl_2 phase for 12hrs.



Scheme S3 Force balance of a crystal at the interface between H_2O and CH_2Cl_2

We regard the crystal as a cuboid whose edge lengths are a, b, c, for simplicity. Because the crystal is hydrophilic, it exhibits contact angles between 0 and 90° at the interface (θ_1, viewed from a axis, θ_2 viewed from b axis) [S2]. For a static crystal, the vertical component of the surface tension equals to the gravity, so we get:

$$2*(\gamma_{H2O}- \gamma_{CH2Cl2})*a*\cos\theta_1 + 2*(\gamma_{H2O}- \gamma_{CH2Cl2})*b*\cos\theta_2 =\rho*a*b*c*g,$$

where γ_{H2O} and γ_{CH2Cl2} are the sufaces tensions of water and dichloromethane, respectively, ρ is the mass density of the crystal, g is the gravity coefficient.The left side which stands for the total vertical component of the surface tension increases linearly with the crystal size, while the right side which stands for the gravity is proportional to the cube of the size.

At first, the gravity is very tiny and $\theta_{1(2)}$ is nearly 90°. As the crystal size grows, the $\theta_{1(2)}$ should also increase. Finally when $\theta_{1(2)}$ approaches zero, namely, $2*(\gamma_{H2O}- \gamma_{CH2Cl2})*a + 2*(\gamma_{H2O}- \gamma_{CH2Cl2})*b =\rho*a*b*c*g$, the crystal can no longer maintain static at the interface and then falls to the bottom.

Reference

S2 L. L. Schramm, *Emulsions, Foams, and Suspensions: Fundamentals and Applications*, Wiley-VCH Verlag GmbH & Co. KgaA, Weinhiem, **2005**.

3. Diffuse Reflectance Spectra of 1~4

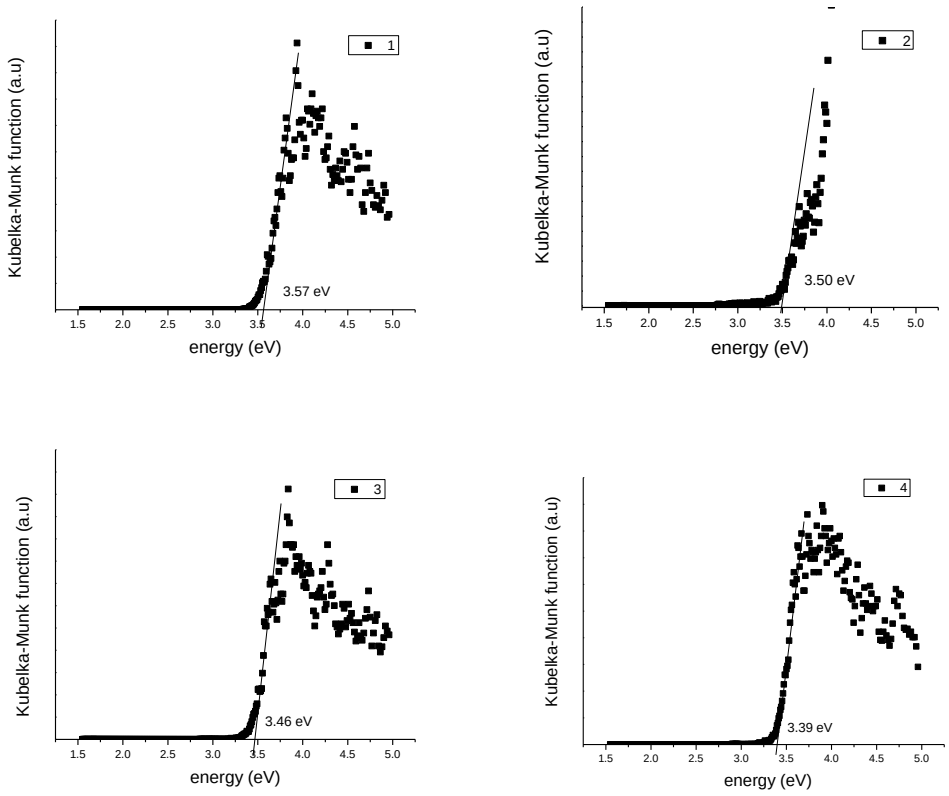


Fig S3 Diffuse reflectance spectra and band gap extrapolations of **1~4**.

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5 Crystal Structures of 1~4

1 Crystal Structure of $4[Ag_4I_8]\cdot16[(C_2H_5)_3N(C_7H_6Cl)]\cdot CH_2Cl_2$

The room temperature (295±2°K) single-crystal X-ray experiments were performed on a Rigaku RAXIS-RAPID diffractometer with monochromatized Mo K_α radiation. Unit cell was obtained and refined by 48955 well centered reflections with $3.0°<\theta< 25.5°$. No decay was observed except the statistic fluctuation. Raw intensities were corrected for Lorentz and polarization effects, and for absorption by empirical method. Direct phase determination yielded the positions of all Ag and I atoms. The other non-hydrogen atoms were located in the successive Fourier syntheses. All non-hydrogen atoms were subjected to anisotropic refinement. The sample is a twin crystal. The disordered solvent molecule, CH_2Cl_2, was found in the hole. Its occupancy was fixed to be 0.5 in the final refinement according to the refinement for the occupancy before. All hydrogen atoms were generated geometically with C-H bond distances of 0.93-0.97 Å according to criteria described in the SHELXTL manual (Bruker, 1997). They were included in the refinement with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(methyl C). The final full-matric least-square refinement on F^2 converged with $R1 = 0.0867$ and $wR2 = 0.1897$ for 19314 observed reflections [$I \geq 2\sigma(I)$]. The final difference electron density map shows no features. Details of crystal parameters, data collection and structure refinement are given in Table 1.

Data collection was controlled by Crystalclear program. Computations were performed using the SHELXTL NT ver. 5.10 program package (Bruker, 1997) on a IBM PC 586 computer. Analytic expressions of atomic scattering factors were employed, and anomalous dispersion corrections were incorporated (*International Tables for X-ray Crystallography*, 1989). Crystal drawing were produced with XP (Bruker, 1998).

References

Bruker.(1997) SHELXTL. Structure Determination Programs, Version 5.10, Bruker AXS Inc.,6300 Enterprise Lane, Madison, WI 53719-1173, USA.

International Tables for X-ray Crystallography: (1989) Vol. C (Kluwer Academic Publishers, Dordrecht) Tables 4.2.6.8 and 6.1.1.4.

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Table 1. Details of Data Collection, Processing and Structure Refinement

Sample code	**1**
Molecular formula	$4[Ag_4I_8]\cdot16[C_{13}H_{21}ClN]\cdot CH_2Cl_2$
Molecular weight	9499.77
Color and habit	colorless block
Crystal size	0.05 × 0.05 × 0.05 mm
Crystal system	monoclinic
Space group	*Pc* (No. 7)
Unit cell parameters	*a* = 12.263(3) Å α = 90.00° *b* = 24.775(5) Å β = 91.51(3)° *c* = 24.888(5) Å γ = 90.00° *V* = 7559(3) Å^3 *Z* = 1 *F*(000) = 4458
Density (calcd)	2.087 g/cm^3
Diffractometer	Rigaku RAXIS-RAPID
Radiation	graphite-monochromatized Mo K_α, λ = 0.71073 Å
Temperature	295±2K
Scan type	ω-scan
Data collection range	-14 <*h*< 14, -30 <*k*< 29, -30 <*l* < 30; θ_{max} = 25.5°
Reflections measured	Total: 60557 Unique (*n*): 26101 Observed [I ≥ 2σ(I)]: 19314
Absorption coefficient	4.480 mm^{-1}
Minimum and maximum transmission	1.000, 0.036
No. of variables, *p*	1326
Weighting scheme	$w = \frac{1}{\sigma^2(F_o^2) + (0.001P)^2 + 5.0P}$ $P = (F_o^2 + 2F_c^2)/3$
$R1 = \frac{\Sigma\|\|F_o\|-\|F_c\|\|}{\Sigma\|F_o\|}$ (for all reflections)	0.1058 0.0867 (for observed data)
$wR2 = \sqrt{\frac{\Sigma[w(F_o^2 - F_c^2)^2]}{\Sigma w(F_o^2)^2}}$ (for all reflections)	0.2046 0.1897 (for observed data)
Goof = S = $\sqrt{\frac{\Sigma[w(F_o^2 - F_c^2)^2]}{n - p}}$	1.458
Largest and mean Δ/σ	0.018, 0.000
Residual extrema in final difference map	-2.036 to 2.864 *e*Å^{-3}

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Table 2. Atomic coordinates and equivalent isotropic temperature factors* ($Å^2$)

Atoms	*x*	*y*	*z*	$U_{eq.}$
I(1)	0.59169(5)	0.53460(3)	0.22613(3)	0.05199(19)
I(2)	0.23494(6)	0.59373(3)	0.18194(3)	0.0665(2)
I(3)	0.30202(6)	0.40988(3)	0.22433(3)	0.0633(2)
I(4)	0.32087(6)	0.54501(3)	0.35895(3)	0.0580(2)
I(5)	0.20518(6)	0.36998(4)	0.39845(4)	0.0688(2)
I(6)	0.57573(6)	0.40454(3)	0.36013(3)	0.0583(2)
I(7)	0.66652(8)	0.35548(4)	0.18703(4)	0.0783(3)
I(8)	0.66868(6)	0.58365(3)	0.40793(3)	0.0630(2)
I(9)	0.56522(6)	1.03745(3)	0.33919(3)	0.0612(2)
I(10)	0.22477(7)	1.09512(3)	0.38730(3)	0.0694(3)
I(11)	0.29433(6)	0.90689(3)	0.34540(3)	0.0589(2)
I(12)	0.29584(6)	1.03818(3)	0.21082(3)	0.0561(2)
I(13)	0.19485(8)	0.86369(4)	0.16245(4)	0.0858(3)
I(14)	0.55434(7)	0.89843(3)	0.21528(4)	0.0726(3)
I(15)	0.66006(7)	0.85671(4)	0.39229(4)	0.0728(3)
I(16)	0.66230(8)	1.06208(4)	0.15400(4)	0.0892(3)
Ag(1)	0.35420(8)	0.52385(4)	0.24504(4)	0.0741(3)
Ag(2)	0.34543(8)	0.43060(5)	0.33770(4)	0.0749(3)
Ag(3)	0.53396(9)	0.42180(4)	0.24444(4)	0.0757(3)
Ag(4)	0.54623(8)	0.51890(4)	0.33892(4)	0.0704(3)
Ag(5)	0.33382(8)	1.02016(4)	0.32645(4)	0.0724(3)
Ag(6)	0.32746(9)	0.92202(5)	0.23115(5)	0.0822(4)
Ag(7)	0.53052(9)	0.92191(5)	0.32869(5)	0.0843(4)
Ag(8)	0.53032(9)	1.01403(5)	0.22622(5)	0.0810(4)
Cl(1)	1.1799(4)	0.6096(2)	0.48167(19)	0.1346(18)
Cl(2)	0.6670(4)	0.1608(2)	0.4126(3)	0.203(2)
Cl(3)	0.7829(5)	0.3112(3)	0.5768(2)	0.197(3)
Cl(4)	-0.0517(4)	0.1736(3)	0.1627(2)	0.170(2)
Cl(5)	0.9358(3)	0.40510(19)	0.5091(2)	0.1134(16)
Cl(6)	0.1223(4)	1.22876(19)	0.0515(3)	0.157(3)
Cl(7)	1.0972(5)	0.7207(3)	0.3707(3)	0.182(3)
Cl(8)	0.9693(5)	0.8787(2)	0.5124(3)	0.150(2)
N(1)	0.7545(4)	0.7225(2)	0.5206(2)	0.052(3)
N(2)	1.0997(4)	0.2215(2)	0.5041(2)	0.057(3)
N(3)	0.4926(4)	0.28297(18)	0.7687(2)	0.045(2)
N(4)	0.4118(4)	0.22036(19)	0.2573(2)	0.061(3)
N(5)	0.4551(4)	0.4699(2)	0.53922(19)	0.054(3)
N(6)	0.3732(4)	1.0189(2)	0.03087(19)	0.057(3)
N(7)	0.9495(4)	0.5043(2)	0.3007(2)	0.073(3)
N(8)	0.9419(4)	0.9813(2)	0.2887(2)	0.094(4)

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(Table 2. continued)

Atoms	*x*	*y*	*z*	$U_{eq.}$
C(1)	0.7876(8)	0.6671(2)	0.5352(4)	0.050(3)
C(2)	0.9098(7)	0.6589(4)	0.5505(3)	0.061(3)
C(3)	0.9426(9)	0.6625(5)	0.6044(6)	0.075(4)
C(4)	1.0529(11)	0.6516(6)	0.6210(6)	0.087(5)
C(5)	1.1195(10)	0.6331(5)	0.5827(6)	0.076(4)
C(6)	1.0857(9)	0.6285(6)	0.5303(5)	0.072(4)
C(7)	0.9838(7)	0.6397(4)	0.5138(4)	0.058(3)
C(8)	0.8253(7)	0.7484(3)	0.4811(2)	0.061(3)
C(9)	0.8242(12)	0.7229(4)	0.4246(3)	0.085(5)
C(10)	0.7604(9)	0.7542(3)	0.5705(3)	0.074(4)
C(11)	0.7098(11)	0.8112(3)	0.5664(6)	0.114(6)
C(12)	0.6426(4)	0.7207(4)	0.4979(3)	0.062(4)
C(13)	0.5557(8)	0.7064(7)	0.5393(5)	0.128(7)
C(14)	1.0666(11)	0.2247(5)	0.4465(3)	0.079(4)
C(15)	0.9483(10)	0.2370(5)	0.4335(5)	0.070(4)
C(16)	0.9163(9)	0.2899(5)	0.4244(5)	0.065(4)
C(17)	0.8132(11)	0.3046(5)	0.4134(5)	0.074(4)
C(18)	0.7319(12)	0.2654(6)	0.4100(6)	0.090(5)
C(19)	0.7646(12)	0.2089(5)	0.4193(6)	0.086(5)
C(20)	0.8762(10)	0.1978(6)	0.4279(6)	0.089(4)
C(21)	1.0859(9)	0.2763(3)	0.5262(3)	0.073(4)
C(22)	1.1326(13)	0.2861(5)	0.5830(3)	0.108(6)
C(23)	1.0281(7)	0.1848(2)	0.5334(4)	0.063(4)
C(24)	1.0339(11)	0.1237(3)	0.5213(6)	0.077(4)
C(25)	1.2142(4)	0.2035(3)	0.5076(4)	0.058(3)
C(26)	1.3052(7)	0.2393(4)	0.4860(6)	0.108(5)
C(27)	0.4854(8)	0.3150(3)	0.7192(3)	0.044(2)
C(28)	0.5221(9)	0.2899(4)	0.6690(5)	0.059(3)
C(29)	0.4691(9)	0.2487(4)	0.6419(3)	0.075(4)
C(30)	0.5080(14)	0.2267(6)	0.5949(4)	0.136(8)
C(31)	0.6100(9)	0.2461(4)	0.5753(5)	0.099(4)
C(32)	0.6692(10)	0.2855(4)	0.6036(5)	0.082(4)
C(33)	0.6212(10)	0.3083(5)	0.6482(5)	0.075(4)
C(34)	0.4163(5)	0.2372(3)	0.7684(5)	0.068(4)
C(35)	0.2943(6)	0.2520(6)	0.7633(6)	0.095(5)
C(36)	0.6019(4)	0.2596(3)	0.7779(5)	0.068(3)
C(37)	0.6945(7)	0.3010(4)	0.7865(5)	0.093(5)
C(38)	0.4687(11)	0.3220(3)	0.8116(2)	0.075(4)
C(39)	0.4635(13)	0.2991(5)	0.8689(3)	0.105(5)

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(Table 2. continued)

Atoms	*x*	*y*	*z*	$U_{eq.}$
C(40)	0.3183(6)	0.1859(4)	0.2695(5)	0.062(3)
C(41)	0.1995(9)	0.2084(3)	0.2592(4)	0.075(4)
C(42)	0.1347(14)	0.1891(5)	0.2180(6)	0.102(6)
C(43)	0.0293(13)	0.2083(7)	0.2117(8)	0.121(6)
C(44)	-0.0090(13)	0.2482(8)	0.2444(8)	0.113(6)
C(45)	0.0587(14)	0.2680(7)	0.2829(7)	0.104(6)
C(46)	0.1610(9)	0.2493(4)	0.2917(5)	0.085(4)
C(47)	0.4251(11)	0.2673(3)	0.2934(2)	0.076(4)
C(48)	0.4283(14)	0.2513(5)	0.3532(3)	0.099(5)
C(49)	0.5008(5)	0.1811(3)	0.2630(6)	0.091(5)
C(50)	0.6164(6)	0.2042(6)	0.2558(8)	0.126(8)
C(51)	0.4106(11)	0.2416(4)	0.2022(2)	0.102(6)
C(52)	0.4032(18)	0.2029(5)	0.1539(4)	0.160(9)
C(53)	0.5455(5)	0.4898(4)	0.5070(3)	0.045(3)
C(54)	0.6592(9)	0.4852(5)	0.5326(5)	0.062(4)
C(55)	0.7389(10)	0.4501(5)	0.5135(5)	0.068(4)
C(56)	0.8442(9)	0.4493(5)	0.5313(5)	0.064(4)
C(57)	0.8773(11)	0.4886(6)	0.5649(6)	0.089(5)
C(58)	0.8025(9)	0.5249(5)	0.5872(6)	0.077(4)
C(59)	0.6931(10)	0.5245(4)	0.5686(5)	0.070(4)
C(60)	0.4712(10)	0.4151(2)	0.5607(3)	0.073(4)
C(61)	0.4788(12)	0.3716(4)	0.5173(4)	0.102(6)
C(62)	0.4385(9)	0.5051(2)	0.5857(3)	0.067(4)
C(63)	0.4206(12)	0.5658(3)	0.5758(6)	0.095(5)
C(64)	0.3558(4)	0.4738(5)	0.5047(3)	0.069(4)
C(65)	0.2478(7)	0.4590(6)	0.5315(5)	0.100(6)
C(66)	0.3879(9)	1.0701(3)	0.0609(4)	0.054(3)
C(67)	0.3570(8)	1.1207(4)	0.0321(4)	0.049(3)
C(68)	0.2642(9)	1.1471(5)	0.0506(5)	0.065(4)
C(69)	0.2333(12)	1.1949(5)	0.0285(7)	0.104(6)
C(70)	0.2903(15)	1.2126(5)	-0.0145(7)	0.116(6)
C(71)	0.3906(15)	1.1912(7)	-0.0301(7)	0.133(7)
C(72)	0.4165(11)	1.1454(5)	-0.0071(5)	0.070(4)
C(73)	0.2606(4)	1.0124(4)	0.0098(3)	0.061(3)
C(74)	0.1747(7)	1.0092(5)	0.0536(4)	0.075(4)
C(75)	0.4034(9)	0.9748(2)	0.0680(3)	0.061(3)
C(76)	0.3978(13)	0.9159(3)	0.0478(5)	0.084(5)
C(77)	0.4393(5)	1.0180(4)	-0.0183(3)	0.058(3)
C(78)	0.5643(6)	1.0197(5)	-0.0102(5)	0.084(4)

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(Table 2. continued)

Atoms	*x*	*y*	*z*	$U_{eq.}$
C(79)	0.8819(7)	0.5528(3)	0.2978(6)	0.091(5)
C(80)	0.9404(11)	0.6089(5)	0.2892(3)	0.091(4)
C(81)	0.9859(8)	0.6362(3)	0.3330(6)	0.094(6)
C(82)	1.0382(10)	0.6837(4)	0.3194(7)	0.108(6)
C(83)	1.0250(13)	0.7087(8)	0.2693(10)	0.142(9)
C(84)	0.9769(12)	0.6828(3)	0.2267(8)	0.129(8)
C(85)	0.9340(11)	0.6321(4)	0.2382(4)	0.121(7)
C(86)	1.0202(7)	0.5055(7)	0.3494(2)	0.119(6)
C(87)	0.9659(10)	0.5057(8)	0.4044(3)	0.144(8)
C(88)	0.8659(6)	0.4630(2)	0.3071(7)	0.115(6)
C(89)	0.9123(12)	0.4055(3)	0.3042(9)	0.176(9)
C(90)	1.0277(6)	0.4965(6)	0.2576(2)	0.090(5)
C(91)	0.9705(10)	0.4897(7)	0.2021(3)	0.110(6)
C(92)	1.0078(8)	0.9872(5)	0.3382(4)	0.137(9)
C(93)	0.9562(9)	0.9843(7)	0.3904(7)	0.091(5)
C(94)	0.9803(11)	0.9371(6)	0.4269(7)	0.090(5)
C(95)	0.9312(13)	0.9342(7)	0.4743(7)	0.121(5)
C(96)	0.8605(13)	0.9674(9)	0.5007(9)	0.145(9)
C(97)	0.8421(10)	1.0122(7)	0.4659(3)	0.117(6)
C(98)	0.8867(10)	1.0210(8)	0.4157(4)	0.132(8)
C(99)	0.8814(7)	0.9311(2)	0.2954(6)	0.117(6)
C(100)	0.9495(11)	0.8795(4)	0.2886(9)	0.153(9)
C(101)	1.0169(6)	0.9877(6)	0.2445(2)	0.097(6)
C(102)	0.9641(10)	0.9833(8)	0.1878(3)	0.157(8)
C(103)	0.8548(6)	1.0215(2)	0.2860(8)	0.137(8)
C(104)	0.9002(14)	1.0794(4)	0.2872(10)	0.177(12)
Cl(9)	0.7250(6)	0.1192(3)	0.5486(3)	0.116(3)
Cl(10)	0.8343(7)	0.1600(3)	0.6437(3)	0.131(4)
C(105)	0.7842(12)	0.1049(4)	0.6099(4)	0.219(14)

*$U_{eq.}$defined as one third of the trace of the orthogonalized**U** tensor.

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Table 3. Bond lengths (Å) and bond angles (°)

I(1)-Ag(4)	2.9024(14)	N(1)-C(12)	1.470(7)
I(1)-Ag(3)	2.9216(14)	N(1)-C(1)	1.474(7)
I(1)-Ag(1)	2.9743(14)	N(1)-C(8)	1.476(7)
I(2)-Ag(1)	2.7352(14)	N(2)-C(23)	1.470(7)
I(3)-Ag(3)	2.8900(14)	N(2)-C(25)	1.473(7)
I(3)-Ag(2)	2.9033(15)	N(2)-C(21)	1.476(7)
I(3)-Ag(1)	2.9378(15)	N(2)-C(14)	1.484(7)
I(4)-Ag(4)	2.8944(13)	N(3)-C(27)	1.467(7)
I(4)-Ag(2)	2.9005(15)	N(3)-C(34)	1.470(7)
I(4)-Ag(1)	2.9224(15)	N(3)-C(36)	1.472(7)
I(5)-Ag(2)	2.7636(15)	N(3)-C(38)	1.475(7)
I(6)-Ag(4)	2.9031(14)	N(4)-C(49)	1.466(7)
I(6)-Ag(2)	2.9362(14)	N(4)-C(40)	1.467(7)
I(6)-Ag(3)	2.9425(15)	N(4)-C(51)	1.468(7)
I(7)-Ag(3)	2.7398(15)	N(4)-C(47)	1.474(7)
I(8)-Ag(4)	2.7645(14)	N(5)-C(62)	1.468(7)
I(9)-Ag(5)	2.8790(14)	N(5)-C(53)	1.470(7)
I(9)-Ag(8)	2.8914(15)	N(5)-C(60)	1.471(7)
I(9)-Ag(7)	2.9046(16)	N(5)-C(64)	1.475(7)
I(10)-Ag(5)	2.7637(14)	N(6)-C(75)	1.472(7)
I(11)-Ag(5)	2.8886(14)	N(6)-C(73)	1.473(7)
I(11)-Ag(6)	2.9073(15)	N(6)-C(66)	1.483(7)
I(11)-Ag(7)	2.9605(15)	N(6)-C(77)	1.485(7)
I(12)-Ag(5)	2.9371(14)	N(7)-C(88)	1.460(7)
I(12)-Ag(6)	2.9460(15)	N(7)-C(79)	1.462(8)
I(12)-Ag(8)	2.9521(15)	N(7)-C(86)	1.470(7)
I(13)-Ag(6)	2.7403(16)	N(7)-C(90)	1.471(7)
I(14)-Ag(6)	2.8803(16)	N(8)-C(103)	1.460(7)
I(14)-Ag(8)	2.8927(15)	N(8)-C(101)	1.461(7)
I(14)-Ag(7)	2.9043(16)	N(8)-C(99)	1.462(7)
I(15)-Ag(7)	2.7396(16)	N(8)-C(92)	1.463(8)
I(16)-Ag(8)	2.7243(16)	C(1)-C(2)	1.550(13)
Cl(1)-C(6)	1.758(13)	C(2)-C(7)	1.389(8)
Cl(2)-C(19)	1.693(14)	C(2)-C(3)	1.391(16)
Cl(3)-C(32)	1.687(14)	C(3)-C(4)	1.429(17)
Cl(4)-C(43)	1.774(18)	C(4)-C(5)	1.352(19)
Cl(5)-C(56)	1.673(12)	C(5)-C(6)	1.363(18)
Cl(6)-C(69)	1.711(15)	C(6)-C(7)	1.334(14)
Cl(7)-C(82)	1.717(17)	C(8)-C(9)	1.541(8)
Cl(8)-C(95)	1.728(17)	C(10)-C(11)	1.543(8)
N(1)-C(10)	1.470(7)	C(12)-C(13)	1.542(8)

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(Table 3. continued)

C(14)-C(15)	1.508(17)	C(58)-C(59)	1.407(17)
C(15)-C(20)	1.319(17)	C(60)-C(61)	1.531(8)
C(15)-C(16)	1.385(17)	C(62)-C(63)	1.538(7)
C(16)-C(17)	1.337(17)	C(64)-C(65)	1.544(8)
C(17)-C(18)	1.392(18)	C(66)-C(67)	1.487(13)
C(18)-C(19)	1.474(18)	C(67)-C(72)	1.378(16)
C(19)-C(20)	1.407(18)	C(67)-C(68)	1.401(15)
C(21)-C(22)	1.531(8)	C(68)-C(69)	1.357(18)
C(23)-C(24)	1.546(7)	C(69)-C(70)	1.37(2)
C(25)-C(26)	1.534(8)	C(70)-C(71)	1.40(2)
C(27)-C(28)	1.475(14)	C(71)-C(72)	1.31(2)
C(28)-C(29)	1.377(14)	C(73)-C(74)	1.538(8)
C(28)-C(33)	1.408(17)	C(75)-C(76)	1.544(7)
C(29)-C(30)	1.388(9)	C(77)-C(78)	1.541(7)
C(30)-C(31)	1.44(2)	C(79)-C(80)	1.579(15)
C(31)-C(32)	1.395(9)	C(80)-C(81)	1.387(16)
C(32)-C(33)	1.390(17)	C(80)-C(85)	1.394(8)
C(34)-C(35)	1.542(8)	C(81)-C(82)	1.386(9)
C(36)-C(37)	1.540(8)	C(82)-C(83)	1.40(3)
C(38)-C(39)	1.537(8)	C(83)-C(84)	1.36(3)
C(40)-C(41)	1.575(14)	C(84)-C(85)	1.394(9)
C(41)-C(42)	1.367(17)	C(86)-C(87)	1.538(8)
C(41)-C(46)	1.387(8)	C(88)-C(89)	1.537(8)
C(42)-C(43)	1.38(2)	C(90)-C(91)	1.541(8)
C(43)-C(44)	1.37(3)	C(92)-C(93)	1.461(19)
C(44)-C(45)	1.34(2)	C(93)-C(98)	1.41(2)
C(45)-C(46)	1.35(2)	C(93)-C(94)	1.51(2)
C(47)-C(48)	1.540(8)	C(94)-C(95)	1.34(2)
C(49)-C(50)	1.544(8)	C(95)-C(96)	1.37(3)
C(51)-C(52)	1.538(8)	C(96)-C(97)	1.42(3)
C(53)-C(54)	1.522(14)	C(97)-C(98)	1.393(9)
C(54)-C(59)	1.381(16)	C(99)-C(100)	1.538(9)
C(54)-C(55)	1.401(16)	C(101)-C(102)	1.541(8)
C(55)-C(56)	1.354(17)	C(103)-C(104)	1.539(8)
C(56)-C(57)	1.340(19)	Cl(10)-C(105)	1.711(8)
C(57)-C(58)	1.411(19)		

Ag(4)-I(1)-Ag(3)	70.58(3)	Ag(3)-I(3)-Ag(1)	70.28(3)
Ag(4)-I(1)-Ag(1)	67.73(4)	Ag(2)-I(3)-Ag(1)	68.04(4)
Ag(3)-I(1)-Ag(1)	69.35(3)	Ag(4)-I(4)-Ag(2)	69.26(3)
Ag(3)-I(3)-Ag(2)	70.08(4)	Ag(4)-I(4)-Ag(1)	68.54(4)

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(Table 3. continued)

Ag(2)-I(4)-Ag(1)	68.28(4)	I(10)-Ag(5)-I(9)	109.24(5)
Ag(4)-I(6)-Ag(2)	68.66(3)	I(10)-Ag(5)-I(11)	118.53(5)
Ag(4)-I(6)-Ag(3)	70.27(3)	I(9)-Ag(5)-I(11)	107.19(4)
Ag(2)-I(6)-Ag(3)	68.92(4)	I(10)-Ag(5)-I(12)	111.61(4)
Ag(5)-I(9)-Ag(8)	75.10(5)	I(9)-Ag(5)-I(12)	102.45(5)
Ag(5)-I(9)-Ag(7)	72.65(4)	I(11)-Ag(5)-I(12)	106.55(4)
Ag(8)-I(9)-Ag(7)	72.38(4)	I(13)-Ag(6)-I(14)	111.53(5)
Ag(5)-I(11)-Ag(6)	71.74(4)	I(13)-Ag(6)-I(11)	116.51(5)
Ag(5)-I(11)-Ag(7)	71.70(4)	I(14)-Ag(6)-I(11)	105.57(5)
Ag(6)-I(11)-Ag(7)	71.57(5)	I(13)-Ag(6)-I(12)	109.56(5)
Ag(5)-I(12)-Ag(6)	70.52(3)	I(14)-Ag(6)-I(12)	107.33(4)
Ag(5)-I(12)-Ag(8)	73.34(4)	I(11)-Ag(6)-I(12)	105.82(4)
Ag(6)-I(12)-Ag(8)	69.90(4)	I(15)-Ag(7)-I(14)	111.82(5)
Ag(6)-I(14)-Ag(8)	71.65(4)	I(15)-Ag(7)-I(9)	116.60(5)
Ag(6)-I(14)-Ag(7)	72.77(5)	I(14)-Ag(7)-I(9)	105.46(5)
Ag(8)-I(14)-Ag(7)	72.36(4)	I(15)-Ag(7)-I(11)	113.53(5)
I(2)-Ag(1)-I(4)	110.92(5)	I(14)-Ag(7)-I(11)	103.61(5)
I(2)-Ag(1)-I(3)	113.39(5)	I(9)-Ag(7)-I(11)	104.64(4)
I(4)-Ag(1)-I(3)	107.89(4)	I(16)-Ag(8)-I(9)	118.60(5)
I(2)-Ag(1)-I(1)	111.31(5)	I(16)-Ag(8)-I(14)	107.87(5)
I(4)-Ag(1)-I(1)	107.46(5)	I(9)-Ag(8)-I(14)	106.11(4)
I(3)-Ag(1)-I(1)	105.54(4)	I(16)-Ag(8)-I(12)	114.79(5)
I(5)-Ag(2)-I(4)	111.24(5)	I(9)-Ag(8)-I(12)	101.78(5)
I(5)-Ag(2)-I(3)	109.56(5)	I(14)-Ag(8)-I(12)	106.84(4)
I(4)-Ag(2)-I(3)	109.44(4)	C(10)-N(1)-C(12)	111.4(6)
I(5)-Ag(2)-I(6)	112.69(5)	C(10)-N(1)-C(1)	106.4(6)
I(4)-Ag(2)-I(6)	106.52(4)	C(12)-N(1)-C(1)	108.4(6)
I(3)-Ag(2)-I(6)	107.26(5)	C(10)-N(1)-C(8)	108.3(6)
I(7)-Ag(3)-I(3)	116.31(5)	C(12)-N(1)-C(8)	108.4(6)
I(7)-Ag(3)-I(1)	110.04(5)	C(1)-N(1)-C(8)	114.0(6)
I(3)-Ag(3)-I(1)	108.19(4)	C(23)-N(2)-C(25)	111.4(6)
I(7)-Ag(3)-I(6)	109.44(5)	C(23)-N(2)-C(21)	107.9(6)
I(3)-Ag(3)-I(6)	107.44(5)	C(25)-N(2)-C(21)	112.0(7)
I(1)-Ag(3)-I(6)	104.78(4)	C(23)-N(2)-C(14)	111.1(7)
I(8)-Ag(4)-I(4)	105.59(4)	C(25)-N(2)-C(14)	108.0(7)
I(8)-Ag(4)-I(1)	114.08(4)	C(21)-N(2)-C(14)	106.3(6)
I(4)-Ag(4)-I(1)	110.20(5)	C(27)-N(3)-C(34)	112.9(7)
I(8)-Ag(4)-I(6)	112.97(4)	C(27)-N(3)-C(36)	112.2(7)
I(4)-Ag(4)-I(6)	107.56(4)	C(34)-N(3)-C(36)	105.9(5)
I(1)-Ag(4)-I(6)	106.29(4)	C(27)-N(3)-C(38)	104.1(5)

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(Table 3. continued)

C(34)-N(3)-C(38)	111.7(7)	C(7)-C(6)-Cl(1)	118.2(9)
C(36)-N(3)-C(38)	110.1(7)	C(5)-C(6)-Cl(1)	119.5(9)
C(49)-N(4)-C(40)	100.2(5)	C(6)-C(7)-C(2)	119.5(10)
C(49)-N(4)-C(51)	108.5(8)	N(1)-C(8)-C(9)	116.0(7)
C(40)-N(4)-C(51)	114.4(8)	N(1)-C(10)-C(11)	115.0(7)
C(49)-N(4)-C(47)	113.2(7)	N(1)-C(12)-C(13)	113.9(7)
C(40)-N(4)-C(47)	114.0(7)	N(2)-C(14)-C(15)	117.1(9)
C(51)-N(4)-C(47)	106.5(5)	C(20)-C(15)-C(16)	119.6(11)
C(62)-N(5)-C(53)	110.7(6)	C(20)-C(15)-C(14)	120.8(11)
C(62)-N(5)-C(60)	106.4(5)	C(16)-C(15)-C(14)	119.5(11)
C(53)-N(5)-C(60)	114.3(7)	C(17)-C(16)-C(15)	123.6(12)
C(62)-N(5)-C(64)	106.9(7)	C(16)-C(17)-C(18)	119.7(12)
C(53)-N(5)-C(64)	106.5(5)	C(17)-C(18)-C(19)	117.5(12)
C(60)-N(5)-C(64)	111.9(7)	C(20)-C(19)-C(18)	118.0(12)
C(75)-N(6)-C(73)	111.2(7)	C(20)-C(19)-Cl(2)	124.1(10)
C(75)-N(6)-C(66)	107.1(5)	C(18)-C(19)-Cl(2)	117.6(11)
C(73)-N(6)-C(66)	111.9(7)	C(15)-C(20)-C(19)	121.2(12)
C(75)-N(6)-C(77)	111.9(6)	N(2)-C(21)-C(22)	116.5(7)
C(73)-N(6)-C(77)	103.4(5)	N(2)-C(23)-C(24)	118.5(7)
C(66)-N(6)-C(77)	111.5(7)	N(2)-C(25)-C(26)	120.4(7)
C(88)-N(7)-C(79)	100.5(6)	N(3)-C(27)-C(28)	118.0(7)
C(88)-N(7)-C(86)	109.0(9)	C(29)-C(28)-C(33)	117.4(11)
C(79)-N(7)-C(86)	110.2(9)	C(29)-C(28)-C(27)	125.1(10)
C(88)-N(7)-C(90)	117.4(8)	C(33)-C(28)-C(27)	117.4(10)
C(79)-N(7)-C(90)	116.8(8)	C(28)-C(29)-C(30)	122.4(12)
C(86)-N(7)-C(90)	102.8(5)	C(29)-C(30)-C(31)	118.5(12)
C(103)-N(8)-C(101)	111.5(10)	C(32)-C(31)-C(30)	120.5(11)
C(103)-N(8)-C(99)	102.3(5)	C(33)-C(32)-C(31)	117.5(12)
C(101)-N(8)-C(99)	120.7(9)	C(33)-C(32)-Cl(3)	122.2(9)
C(103)-N(8)-C(92)	111.0(10)	C(31)-C(32)-Cl(3)	119.3(10)
C(101)-N(8)-C(92)	106.2(6)	C(32)-C(33)-C(28)	123.4(12)
C(99)-N(8)-C(92)	105.0(8)	N(3)-C(34)-C(35)	115.7(7)
N(1)-C(1)-C(2)	116.1(7)	N(3)-C(36)-C(37)	115.1(6)
C(7)-C(2)-C(3)	118.6(9)	N(3)-C(38)-C(39)	116.3(7)
C(7)-C(2)-C(1)	121.8(8)	N(4)-C(40)-C(41)	119.1(7)
C(3)-C(2)-C(1)	118.8(8)	C(42)-C(41)-C(46)	119.6(12)
C(2)-C(3)-C(4)	120.9(12)	C(42)-C(41)-C(40)	121.0(10)
C(5)-C(4)-C(3)	116.4(13)	C(46)-C(41)-C(40)	119.4(10)
C(4)-C(5)-C(6)	121.9(12)	C(41)-C(42)-C(43)	119.2(14)
C(7)-C(6)-C(5)	122.3(11)	C(44)-C(43)-C(42)	121.0(16)

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(Table 3. continued)

C(44)-C(43)-Cl(4)	124.2(13)	N(6)-C(73)-C(74)	114.0(6)
C(42)-C(43)-Cl(4)	114.6(13)	N(6)-C(75)-C(76)	119.2(7)
C(45)-C(44)-C(43)	118.1(16)	N(6)-C(77)-C(78)	117.1(7)
C(44)-C(45)-C(46)	123.0(16)	N(7)-C(79)-C(80)	118.1(8)
C(45)-C(46)-C(41)	119.0(12)	C(81)-C(80)-C(85)	121.6(11)
N(4)-C(47)-C(48)	112.7(7)	C(81)-C(80)-C(79)	119.9(9)
N(4)-C(49)-C(50)	115.2(7)	C(85)-C(80)-C(79)	118.1(10)
N(4)-C(51)-C(52)	120.4(8)	C(82)-C(81)-C(80)	113.7(13)
N(5)-C(53)-C(54)	116.3(8)	C(81)-C(82)-C(83)	123.4(16)
C(59)-C(54)-C(55)	117.3(11)	C(81)-C(82)-Cl(7)	117.4(13)
C(59)-C(54)-C(53)	118.3(10)	C(83)-C(82)-Cl(7)	117.6(10)
C(55)-C(54)-C(53)	122.9(11)	C(84)-C(83)-C(82)	121.5(17)
C(56)-C(55)-C(54)	124.4(12)	C(83)-C(84)-C(85)	115.1(17)
C(57)-C(56)-C(55)	117.7(11)	C(84)-C(85)-C(80)	123.1(13)
C(57)-C(56)-Cl(5)	119.1(10)	N(7)-C(86)-C(87)	118.3(7)
C(55)-C(56)-Cl(5)	123.0(10)	N(7)-C(88)-C(89)	112.5(8)
C(56)-C(57)-C(58)	121.3(12)	N(7)-C(90)-C(91)	112.2(7)
C(59)-C(58)-C(57)	119.4(12)	C(93)-C(92)-N(8)	120.1(9)
C(54)-C(59)-C(58)	119.1(11)	C(98)-C(93)-C(92)	130.4(14)
N(5)-C(60)-C(61)	113.8(6)	C(98)-C(93)-C(94)	110.1(13)
N(5)-C(62)-C(63)	118.4(7)	C(92)-C(93)-C(94)	119.5(13)
N(5)-C(64)-C(65)	115.9(7)	C(95)-C(94)-C(93)	119.1(14)
N(6)-C(66)-C(67)	117.0(7)	C(94)-C(95)-C(96)	133.9(18)
C(72)-C(67)-C(68)	118.5(11)	C(94)-C(95)-Cl(8)	113.8(14)
C(72)-C(67)-C(66)	125.6(10)	C(96)-C(95)-Cl(8)	112.3(15)
C(68)-C(67)-C(66)	115.7(10)	C(95)-C(96)-C(97)	105.5(18)
C(69)-C(68)-C(67)	119.6(12)	C(98)-C(97)-C(96)	127.4(16)
C(68)-C(69)-C(70)	117.1(13)	C(97)-C(98)-C(93)	123.9(16)
C(68)-C(69)-Cl(6)	120.5(13)	N(8)-C(99)-C(100)	114.6(8)
C(70)-C(69)-Cl(6)	122.2(12)	N(8)-C(101)-C(102)	115.1(7)
C(69)-C(70)-C(71)	124.5(14)	N(8)-C(103)-C(104)	111.8(8)
C(72)-C(71)-C(70)	114.3(15)	Cl(9)-C(105)-Cl(10)	114.3(7)
C(71)-C(72)-C(67)	124.7(14)		

Electronic Supplementary Material (ESI) for Nanoscale
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2 Crystal Structure of $[Ag_4I_8]\cdot 4[(C_2H_5)_3(C_7H_7)N]$

The room temperature (295±1°K) single-crystal X-ray experiments were performed on a Rigaku RAXIS-RAPID diffractometer equipped with graphite monochromatized Mo K_α radiation. Unit cell was obtained and refined by 7683 well centered reflections with $2.5° < \theta < 27.5°$. Raw intensities were corrected for Lorentz and polarization effects, and for absorption by empirical method. Direct phase determination yielded the positions of all non-hydrogen atoms. All non-hydrogen atoms were subjected to anisotropic refinement. All hydrogen atoms were generated geometically with C-H bond distances of 0.93-0.97 Å according to criteria described in the SHELXTL manual (Bruker, 1997). They were included in the refinement with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(methyl C). The final full-matric least-square refinement on F^2 converged with $R1 = 0.0547$ and $wR2 = 0.1044$ for 4281 observed reflections [$I \geq 2\sigma(I)$]. The final difference electron density map shows no features. Details of crystal parameters, data collection and structure refinement are given in Table 1.

Data collection was controlled by Crystalclear program. Computations were performed using the SHELXTL NT ver. 5.10 program package (Bruker, 1997) on a IBM PC 586 computer. Analytic expressions of atomic scattering factors were employed, and anomalous dispersion corrections were incorporated (*International Tables for X-ray Crystallography*, 1989). Crystal drawing were produced with XP (Bruker, 1998).

References

Bruker.(1997) SHELXTL. Structure Determination Programs, Version 5.10, Bruker AXS Inc.,6300 Enterprise Lane, Madison, WI53719-1173, USA.

International Tables for X-ray Crystallography: (1989) Vol. C (Kluwer Academic Publishers, Dordrecht) Tables 4.2.6.8 and 6.1.1.4.

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Table 1. Details of Data Collection, Processing and Structure Refinement

Sample code	**2**
Molecular formula	$[Ag_4I_8]\cdot 4[(C_2H_5)_3(C_7H_7)N]$
Molecular weight	2215.94
Color and habit	colorless plate
Crystal size	0.1 × 0.1 ×0.1 mm
Crystal system	triclinic
Space group	$P\bar{1}$ (No. 2)
Unit cell parameters	a = 10.0164(8) Å α = 89.2116(19)° b = 12.4022(9) Å β = 73.399(2)° c = 14.8694(10) Å γ = 73.308(2)° V = 1690.9(2) Å^3 Z = 1 F(000) = 1040
Density (calcd)	2.176 g/cm^3
Diffractometer	Rigaku RAXIS-RAPID
Radiation	graphite-monochromatized Mo K_α, λ = 0.71073 Å
Temperature	295±2K
Scan type	ω-scan
Data collection range	-13 <h< 13, -16 <k< 16, -19 <l < 19; θ_{max} = 27.5°
Reflections measured	Total: 16829 Unique (n): 7683 Observed [I ≥ 2σ(I)]: 4281
Absorption coefficient	4.827 mm^{-1}
Minimum and maximum transmission	0.122, 1.000
No. of variables, p	308
Weighting scheme	$w = \dfrac{1}{\sigma^2(F_o^2) + (0.005P)^2 + 20P}$ $P = (F_o^2 + 2F_c^2)/3$
$R1 = \dfrac{\Sigma\lvert\lvert F_o\rvert - \lvert F_c\rvert\rvert}{\Sigma\lvert F_o\rvert}$ (for all reflections)	0.1152 0.0547 (for observed data)
$wR2 = \sqrt{\dfrac{\Sigma[w(F_o^2 - F_c^2)^2]}{\Sigma w(F_o^2)^2}}$ (for all reflections)	0.1624 0.1044 (for observed data)
Goof = S = $\sqrt{\dfrac{\Sigma[w(F_o^2 - F_c^2)^2]}{n - p}}$	1.223
Largest and mean Δ/σ	0.000, 0.000
Residual extrema in final difference map	-2.471 to 1.817 eÅ^{-3}

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Table 2. Atomic coordinates and equivalent isotropic temperature factors* (Å^2)

Atoms	*x*	*y*	*z*	$U_{eq.}$
Ag(1)	0.93137(13)	0.42069(10)	0.60166(7)	0.0650(3)
Ag(2)	0.80093(13)	0.26857(10)	0.79514(7)	0.0632(3)
I(1)	0.81422(10)	0.49103(7)	0.80363(6)	0.0533(3)
I(2)	0.89995(10)	0.19362(7)	0.60808(6)	0.0546(3)
I(3)	0.78175(10)	0.56243(8)	0.48437(6)	0.0515(3)
I(4)	0.71295(14)	0.16186(9)	0.94931(6)	0.0720(3)
N(1)	0.3057(10)	0.5481(8)	0.8213(6)	0.038(2)
N(2)	0.3185(10)	0.1041(7)	0.2840(6)	0.035(2)
C(1)	0.3140(13)	0.7311(9)	0.7409(8)	0.040(3)
C(2)	0.2129(15)	0.8345(11)	0.7795(9)	0.054(3)
C(3)	0.1617(18)	0.9141(12)	0.7248(11)	0.067(4)
C(4)	0.2069(17)	0.8958(12)	0.6289(12)	0.067(4)
C(5)	0.3096(16)	0.7939(13)	0.5871(10)	0.063(4)
C(6)	0.3627(15)	0.7145(11)	0.6425(8)	0.052(3)
C(7)	0.3709(13)	0.6461(10)	0.8026(9)	0.047(3)
C(8)	0.3701(15)	0.4823(10)	0.8913(8)	0.049(3)
C(9)	0.3214(19)	0.3774(12)	0.9194(10)	0.073(5)
C(10)	0.1410(13)	0.5901(11)	0.8563(8)	0.047(3)
C(11)	0.0766(16)	0.6529(12)	0.9527(9)	0.065(4)
C(12)	0.3417(14)	0.4754(11)	0.7304(7)	0.048(3)
C(13)	0.5002(17)	0.4145(12)	0.6851(9)	0.071(4)
C(14)	0.5383(13)	-0.0745(9)	0.2308(7)	0.038(3)
C(15)	0.6049(16)	-0.1401(10)	0.2932(8)	0.052(3)
C(16)	0.7542(17)	-0.1927(13)	0.2671(10)	0.066(4)
C(17)	0.8384(17)	-0.1810(12)	0.1802(11)	0.063(4)
C(18)	0.7769(16)	-0.1181(12)	0.1159(9)	0.058(4)
C(19)	0.6268(14)	-0.0642(10)	0.1410(8)	0.050(3)
C(20)	0.3787(13)	-0.0226(9)	0.2587(8)	0.041(3)
C(21)	0.3630(15)	0.1703(10)	0.2013(8)	0.049(3)
C(22)	0.3040(18)	0.1576(13)	0.1191(8)	0.069(4)
C(23)	0.3823(14)	0.1345(11)	0.3578(8)	0.048(3)
C(24)	0.3362(17)	0.0901(14)	0.4531(9)	0.071(4)
C(25)	0.1564(12)	0.1321(9)	0.3196(8)	0.040(3)
C(26)	0.0707(13)	0.2562(10)	0.3453(9)	0.052(3)

*$U_{eq.}$ defined as one third of the trace of the orthogonalized **U** tensor.

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Table 3. Bond lengths (Å) and bond angles (°)

Ag(1)-I(3)#1	2.8592(15)	C(1)-C(7)	1.485(16)
Ag(1)-I(3)	2.8764(15)	C(2)-C(3)	1.352(19)
Ag(1)-I(2)	2.9195(15)	C(3)-C(4)	1.37(2)
Ag(1)-I(1)	2.9373(13)	C(4)-C(5)	1.40(2)
Ag(2)-I(4)	2.6862(14)	C(5)-C(6)	1.364(17)
Ag(2)-I(2)	2.7477(14)	C(8)-C(9)	1.529(17)
Ag(2)-I(1)	2.8065(15)	C(10)-C(11)	1.513(16)
I(3)-Ag(1)#1	2.8592(15)	C(12)-C(13)	1.503(18)
N(1)-C(8)	1.491(14)	C(14)-C(19)	1.403(16)
N(1)-C(10)	1.513(15)	C(14)-C(15)	1.411(16)
N(1)-C(7)	1.524(14)	C(14)-C(20)	1.477(16)
N(1)-C(12)	1.530(13)	C(15)-C(16)	1.389(19)
N(2)-C(25)	1.492(14)	C(16)-C(17)	1.36(2)
N(2)-C(21)	1.502(13)	C(17)-C(18)	1.394(19)
N(2)-C(23)	1.519(14)	C(18)-C(19)	1.398(18)
N(2)-C(20)	1.522(14)	C(21)-C(22)	1.530(17)
C(1)-C(2)	1.394(17)	C(23)-C(24)	1.509(17)
C(1)-C(6)	1.400(16)	C(25)-C(26)	1.524(15)

I(3)#1-Ag(1)-I(3)	98.86(4)	C(21)-N(2)-C(20)	112.0(8)
I(3)#1-Ag(1)-I(2)	116.43(5)	C(23)-N(2)-C(20)	108.9(9)
I(3)-Ag(1)-I(2)	113.93(5)	C(2)-C(1)-C(6)	116.9(11)
I(3)#1-Ag(1)-I(1)	114.58(5)	C(2)-C(1)-C(7)	120.4(11)
I(3)-Ag(1)-I(1)	114.94(5)	C(6)-C(1)-C(7)	122.6(11)
I(2)-Ag(1)-I(1)	99.04(4)	C(3)-C(2)-C(1)	121.6(13)
I(4)-Ag(2)-I(2)	130.47(5)	C(2)-C(3)-C(4)	121.0(14)
I(4)-Ag(2)-I(1)	122.84(5)	C(3)-C(4)-C(5)	119.4(13)
I(2)-Ag(2)-I(1)	106.66(4)	C(6)-C(5)-C(4)	119.4(13)
Ag(2)-I(1)-Ag(1)	76.52(4)	C(5)-C(6)-C(1)	121.7(13)
Ag(2)-I(2)-Ag(1)	77.73(4)	C(1)-C(7)-N(1)	116.8(10)
Ag(1)#1-I(3)-Ag(1)	81.14(4)	N(1)-C(8)-C(9)	115.0(11)
C(8)-N(1)-C(10)	112.3(9)	N(1)-C(10)-C(11)	115.7(10)
C(8)-N(1)-C(7)	106.0(9)	C(13)-C(12)-N(1)	116.2(11)
C(10)-N(1)-C(7)	111.2(9)	C(19)-C(14)-C(15)	118.3(11)
C(8)-N(1)-C(12)	111.4(9)	C(19)-C(14)-C(20)	121.4(10)
C(10)-N(1)-C(12)	105.3(9)	C(15)-C(14)-C(20)	120.2(11)
C(7)-N(1)-C(12)	110.8(8)	C(16)-C(15)-C(14)	121.1(12)
C(25)-N(2)-C(21)	110.7(9)	C(17)-C(16)-C(15)	119.8(14)
C(25)-N(2)-C(23)	111.8(8)	C(16)-C(17)-C(18)	120.9(14)
C(21)-N(2)-C(23)	106.1(9)	C(17)-C(18)-C(19)	120.1(13)
C(25)-N(2)-C(20)	107.4(8)	C(18)-C(19)-C(14)	119.7(12)

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(Table 3. continued)

C(14)-C(20)-N(2)	118.4(9)	C(24)-C(23)-N(2)	116.2(10)
N(2)-C(21)-C(22)	115.6(10)	N(2)-C(25)-C(26)	117.0(9)

Symmetry transformation codes: #1 (2-x, 1-y, 1-z).

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3 Crystal Structure of $[Ag_2I_3]\cdot(CH_3)_3N(C_{12}H_{25})$

The room temperature (295±2°K) single-crystal X-ray experiments were performed on a Rigaku RAXIS-RAPID diffractometer with monochromatized Mo K_α radiation. Unit cell was obtained and refined by 6774 well centered reflections with $3.2° < \theta < 27.5°$. No decay was observed except the statistic fluctuation. Raw intensities were corrected for Lorentz and polarization effects, and for absorption by empirical method. Direct phase determination yielded the positions of all Ag and I atoms. The other non-hydrogen atoms were located in the successive Fourier syntheses. All non-hydrogen atoms were subjected to anisotropic refinement. All hydrogen atoms were generated geometically with C-H bond distances of 0.96-0.97 Å according to criteria described in the SHELXTL manual (Bruker, 1997). They were included in the refinement with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(methyl C). The final full-matric least-square refinement on F^2 converged with $R1 = 0.0450$ and $wR2 = 0.0892$ for 2680 observed reflections [$I \geq 2\sigma(I)$]. The final difference electron density map shows no features. Details of crystal parameters, data collection and structure refinement are given in Table 1.

Data collection was controlled by Crystalclear program. Computations were performed using the SHELXTL NT ver. 5.10 program package (Bruker, 1997) on a IBM PC 586 computer. Analytic expressions of atomic scattering factors were employed, and anomalous dispersion corrections were incorporated (*International Tables for X-ray Crystallography*, 1989). Crystal drawing were produced with XP (Bruker, 1998).

References

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International Tables for X-ray Crystallography: (1989) Vol. C (Kluwer Academic Publishers, Dordrecht) Tables 4.2.6.8 and 6.1.1.4.

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Table 1. Details of Data Collection, Processing and Structure Refinement

Sample code	**3**
Molecular formula	$Ag_2I_3 \cdot C_{15}H_{34}N$
Molecular weight	824.87
Color and habit	colorless plate
Crystal size	0.08 × 0.10 ×0.15 mm
Crystal system	triclinic
Space group	$P\bar{1}$ (No. 2)
Unit cell parameters	a = 7.1475(6) Å α = 102.28(2)° b = 9.7391(7) Å β = 98.07(3)° c = 18.189(2) Å γ = 90.85(2)° V = 1223.6(2) Å^3 Z = 2 F(000) = 768
Density (calcd)	2.239 g/cm^3
Diffractometer	Rigaku RAXIS-RAPID
Radiation	graphite-monochromatized Mo K_α, λ = 0.71073 Å
Temperature	295±2K
Scan type	ω-scan
Data collection range	-8 <h< 8, -12 <k< 12, -22 <l < 22; θ_{max} = 26.0°
Reflections measured	Total: 10696 Unique (n): 4785 Observed [I ≥ 2σ(I)]: 2680
Absorption coefficient	5.381 mm^{-1}
Minimum and maximum transmission	1.000, 0.515
No. of variables, p	195
Weighting scheme	$w = \frac{1}{\sigma^2(F_o^2) + (0.001P)^2 + 4.0P}$ $P = (F_o^2 + 2F_c^2)/3$
$R1 = \frac{\Sigma\|\|F_o\|-\|F_c\|\|}{\Sigma\|F_o\|}$ (for all reflections)	0.0940 0.0450 (for observed data)
$wR2 = \sqrt{\frac{\Sigma[w(F_o^2 - F_c^2)^2]}{\Sigma w(F_o^2)^2}}$ (for all reflections)	0.1371 0.0892 (for observed data)
Goof = S = $\sqrt{\frac{\Sigma[w(F_o^2 - F_c^2)^2]}{n - p}}$	1.306
Largest and mean Δ/σ	0.002, 0.000
Residual extrema in final difference map	-1.422 to 1.101 eÅ^{-3}

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Table 2. Atomic coordinates and equivalent isotropic temperature factors* ($Å^2$)

Atoms	*x*	*y*	*z*	$U_{eq.}$
Ag(1)	0.52729(11)	0.96717(8)	0.08500(6)	0.0974(3)
Ag(2)	0.03321(11)	0.96637(8)	0.08310(5)	0.0948(3)
I(1)	0.26968(8)	1.17551(6)	0.04401(4)	0.06994(18)
I(2)	0.28146(8)	0.74866(6)	0.10122(5)	0.0880(2)
I(3)	-0.17368(9)	1.06810(6)	0.20004(4)	0.0773(2)
N(1)	0.8067(9)	0.5311(6)	0.1690(5)	0.071(2)
C(1)	0.6367(12)	0.4658(10)	0.1897(6)	0.084(3)
C(2)	0.6421(12)	0.4585(10)	0.2716(6)	0.086(3)
C(3)	0.4540(13)	0.4026(11)	0.2843(6)	0.089(3)
C(4)	0.4388(14)	0.3879(12)	0.3632(6)	0.098(4)
C(5)	0.2436(15)	0.3417(13)	0.3745(7)	0.115(4)
C(6)	0.2176(16)	0.3189(13)	0.4500(7)	0.113(4)
C(7)	0.0227(15)	0.2747(14)	0.4565(7)	0.117(4)
C(8)	-0.0016(17)	0.2467(14)	0.5339(8)	0.130(5)
C(9)	-0.1934(17)	0.1992(15)	0.5386(6)	0.149(6)
C(10)	-0.2262(13)	0.1655(16)	0.6138(7)	0.172(7)
C(11)	-0.4364(16)	0.1244(16)	0.6106(8)	0.241(11)
C(12)	-0.449(3)	0.059(2)	0.6783(10)	0.280(13)
C(13)	0.7717(18)	0.5273(18)	0.0867(7)	0.155(6)
C(14)	0.9815(14)	0.4578(11)	0.1878(9)	0.141(5)
C(15)	0.8304(18)	0.6825(9)	0.2083(8)	0.134(5)

*$U_{eq.}$ defined as one third of the trace of the orthogonalized **U** tensor.

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Table 3. Bond lengths (Å) and bond angles (°)

Ag(1)-I(3)$^{\#1}$	2.7784(14)	N(1)-C(1)	1.493(11)
Ag(1)-I(2)	2.8293(12)	C(1)-C(2)	1.502(14)
Ag(1)-I(1)	2.9038(12)	C(2)-C(3)	1.509(12)
Ag(1)-I(1)$^{\#2}$	3.0286(14)	C(3)-C(4)	1.491(14)
Ag(2)-I(3)	2.7789(13)	C(4)-C(5)	1.514(14)
Ag(2)-I(2)	2.8280(11)	C(5)-C(6)	1.473(16)
Ag(2)-I(1)	2.8917(12)	C(6)-C(7)	1.479(14)
Ag(2)-I(1)$^{\#3}$	3.0148(14)	C(7)-C(8)	1.524(17)
I(3)-Ag(1)$^{\#4}$	2.7785(14)	C(8)-C(9)	1.460(15)
N(1)-C(13)	1.475(14)	C(9)-C(10)	1.520(9)
N(1)-C(14)	1.482(11)	C(10)-C(11)	1.539(9)
N(1)-C(15)	1.492(10)	C(11)-C(12)	1.514(9)

I(3)$^{\#1}$-Ag(1)-I(2)	119.11(4)	Ag(1)$^{\#4}$-I(3)-Ag(2)	81.32(3)
I(3)$^{\#1}$-Ag(1)-I(1)	115.87(4)	C(13)-N(1)-C(14)	110.1(9)
I(2)-Ag(1)-I(1)	103.23(3)	C(13)-N(1)-C(15)	106.5(10)
I(3)$^{\#1}$-Ag(1)-I(1)$^{\#2}$	102.11(3)	C(14)-N(1)-C(15)	109.9(8)
I(2)-Ag(1)-I(1)$^{\#2}$	102.73(4)	C(13)-N(1)-C(1)	108.0(8)
I(1)-Ag(1)-I(1)$^{\#2}$	113.35(4)	C(14)-N(1)-C(1)	112.3(8)
I(3)-Ag(2)-I(2)	117.82(4)	C(15)-N(1)-C(1)	109.8(8)
I(3)-Ag(2)-I(1)	115.01(4)	N(1)-C(1)-C(2)	117.0(7)
I(2)-Ag(2)-I(1)	103.57(3)	C(1)-C(2)-C(3)	110.3(8)
I(3)-Ag(2)-I(1)$^{\#3}$	102.44(3)	C(4)-C(3)-C(2)	116.4(8)
I(2)-Ag(2)-I(1)$^{\#3}$	103.39(4)	C(3)-C(4)-C(5)	114.5(9)
I(1)-Ag(2)-I(1)$^{\#3}$	114.42(4)	C(6)-C(5)-C(4)	118.1(10)
Ag(2)-I(1)-Ag(1)	74.96(3)	C(5)-C(6)-C(7)	114.8(10)
Ag(2)-I(1)-Ag(2)$^{\#3}$	65.58(4)	C(6)-C(7)-C(8)	114.5(10)
Ag(1)-I(1)-Ag(2)$^{\#3}$	109.26(3)	C(9)-C(8)-C(7)	113.7(10)
Ag(2)-I(1)-Ag(1)$^{\#2}$	108.57(3)	C(8)-C(9)-C(10)	116.4(10)
Ag(1)-I(1)-Ag(1)$^{\#2}$	66.65(4)	C(9)-C(10)-C(11)	109.9(10)
Ag(2)$^{\#3}$-I(1)-Ag(1)$^{\#2}$	73.62(3)	C(12)-C(11)-C(10)	106.4(13)
Ag(2)-I(2)-Ag(1)	77.13(3)		

Symmetry transformation codes: #1 (1+*x*, *y*, *z*); #2 (1-*x*, 2-*y*, -*z*);

#3 (-*x*, 2-*y*, -*z*); #4 (-1+*x*, *y*, *z*).

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4 Crystal Structure of $[Ag_4I_5]\cdot(CH_3)_2N(C_{12}H_{25})_2$

The low temperature (153±2°K) single-crystal X-ray experiments were performed on a Rigaku Saturn70 deffractometer with monochromatized Mo K_α radiation. Unit cell was obtained and refined by 5476 well centered reflections with $1.7°<\theta<25.0°$. No decay was observed except the statistic fluctuation. Raw intensities were corrected for Lorentz and polarization effects, and for absorption by empirical method. Direct phase determination yielded the positions of all Ag and I atoms. The other non-hydrogen atoms were located in the successive Fourier syntheses. All non-hydrogen atoms were subjected to anisotropic refinement. All hydrogen atoms were generated geometically with C-H bond distances of 0.96-0.98 Å according to criteria described in the SHELXTL manual (Bruker, 1997). They were included in the refinement with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(methyl C). The final full-matric least-square refinement on F^2 converged with $R1 = 0.0766$ and $wR2 = 0.1608$ for 3391 observed reflections [$I \geq 2\sigma(I)$]. The final difference electron density map shows no features. Details of crystal parameters, data collection and structure refinement are given in Table 1.

Data collection was controlled by Crystalclear program. Computations were performed using the SHELXTL NT ver. 5.10 program package (Bruker, 1997) on a IBM PC 586 computer. Analytic expressions of atomic scattering factors were employed, and anomalous dispersion corrections were incorporated (*International Tables for X-ray Crystallography*, 1989). Crystal drawing were produced with XP (Bruker, 1998).

References

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International Tables for X-ray Crystallography: (1989) Vol. C (Kluwer Academic Publishers, Dordrecht) Tables 4.2.6.8 and 6.1.1.4.

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Table 1. Details of Data Collection, Processing and Structure Refinement

Sample code	**4**
Molecular formula	$Ag_4I_5 \cdot C_{26}H_{56}N$
Molecular weight	1448.70
Color and habit	colorless plate
Crystal size	0.05 × 0.07 × 0.10 mm
Crystal system	triclinic
Space group	$P\bar{1}$ (No. 2)
Unit cell parameters	a = 9.189(3) Å α = 83.515(13)° b = 10.093(3) Å β = 88.522(13)° c = 23.519(9) Å γ = 68.316(12)° V = 2013.6(11) Å^3 Z = 2 F(000) = 1344
Density (calcd)	2.389 g/cm^3
Diffractometer	Rigaku Saturn70
Radiation	graphite-monochromatized Mo K_α, λ = 0.71073 ?
Temperature	295±2K
Scan type	ω-scan
Data collection range	-10 <h< 10, -12 <k< 11, -28 <l < 28; θ_{max} = 25.0°
Reflections measured	Total: 17431 Unique (n): 6953 Observed [I ≥ 2σ(I)]: 3391
Absorption coefficient	5.766 mm^{-1}
Minimum and maximum transmission	1.000, 0.304
No. of variables, p	326
Weighting scheme	$w = \dfrac{1}{\sigma^2(F_o^2) + (0.001P)^2 + 2.5P}$ $P = (F_o^2 + 2F_c^2)/3$
$R1 = \dfrac{\Sigma\lvert\lvert F_o\rvert - \lvert F_c\rvert\rvert}{\Sigma\lvert F_o\rvert}$ (for all reflections)	0.1034 0.0766 (for observed data)
$wR2 = \sqrt{\dfrac{\Sigma[w(F_o^2 - F_c^2)^2]}{\Sigma w(F_o^2)^2}}$ (for all reflections)	0.1693 0.1608 (for observed data)
Goof = S = $\sqrt{\dfrac{\Sigma[w(F_o^2 - F_c^2)^2]}{n - p}}$	1.277
Largest and mean Δ/σ	0.009, 0.000
Residual extrema in final difference map	-2.160 to 1.989 eÅ^{-3}

Electronic Supplementary Material (ESI) for Nanoscale
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Table 2. Atomic coordinates and equivalent isotropic temperature factors* ($Å^2$)

Atoms	*x*	*y*	*z*	$U_{eq.}$
I(1)	1.25036(9)	-0.02121(8)	1.14280(4)	0.0555(3)
I(2)	1.01285(9)	0.45790(7)	1.14182(4)	0.0499(2)
I(3)	1.39088(9)	0.26138(7)	0.99914(4)	0.0491(2)
I(4)	0.87372(8)	0.24554(7)	0.99957(3)	0.0492(2)
I(5)	0.75256(9)	0.94411(8)	1.13933(4)	0.0546(2)
Ag(1)	1.12742(13)	0.24779(10)	1.06915(5)	0.0721(4)
Ag(2)	0.88165(13)	0.70853(10)	1.07049(5)	0.0726(4)
Ag(3)	1.50651(13)	0.01647(11)	0.93243(5)	0.0788(4)
Ag(4)	0.99852(13)	0.02004(11)	0.92531(5)	0.0750(4)
N(1)	0.4904(9)	0.5383(8)	0.8368(4)	0.039(2)
C(1)	0.4190(11)	0.4547(10)	0.8046(5)	0.042(3)
C(2)	0.5186(11)	0.3806(9)	0.7577(4)	0.035(3)
C(3)	0.4445(13)	0.2934(10)	0.7300(5)	0.058(4)
C(4)	0.5409(14)	0.2075(10)	0.6834(5)	0.061(4)
C(5)	0.5668(14)	0.2994(10)	0.6314(5)	0.060(4)
C(6)	0.6615(14)	0.2123(11)	0.5845(5)	0.061(4)
C(7)	0.6914(15)	0.2933(11)	0.5315(5)	0.064(4)
C(8)	0.7765(15)	0.2072(12)	0.4848(5)	0.072(5)
C(9)	0.8097(15)	0.2896(12)	0.4323(6)	0.073(5)
C(10)	0.8936(14)	0.1995(12)	0.3870(6)	0.066(4)
C(11)	0.9370(16)	0.2730(13)	0.3350(6)	0.088(5)
C(12)	1.0263(17)	0.1777(14)	0.2877(7)	0.109(6)
C(13)	0.5405(11)	0.6430(10)	0.7986(5)	0.043(3)
C(14)	0.4161(13)	0.7468(11)	0.7582(5)	0.053(4)
C(15)	0.4813(16)	0.8296(12)	0.7132(6)	0.077(5)
C(16)	0.5703(15)	0.7355(12)	0.6654(6)	0.078(5)
C(17)	0.6089(14)	0.8125(11)	0.6142(5)	0.060(4)
C(18)	0.6934(15)	0.7208(12)	0.5684(5)	0.066(4)
C(19)	0.7230(16)	0.7992(12)	0.5149(6)	0.078(5)
C(20)	0.8064(14)	0.7118(11)	0.4687(6)	0.064(4)
C(21)	0.8381(15)	0.7889(12)	0.4140(6)	0.071(4)
C(22)	0.9281(15)	0.6984(12)	0.3696(6)	0.072(5)
C(23)	0.9566(17)	0.7751(15)	0.3137(7)	0.096(6)
C(24)	1.0431(16)	0.6814(17)	0.2701(7)	0.126(7)
C(25)	0.6267(12)	0.4400(11)	0.8741(5)	0.061(4)
C(26)	0.3640(12)	0.6227(10)	0.8773(5)	0.055(3)

*$U_{eq.}$ defined as one third of the trace of the orthogonalized **U** tensor.

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Table 3. Bond lengths (Å) and bond angles (°)

I(1)-Ag(4)$^{\#1}$	2.8215(16)	N(1)-C(25)	1.504(11)
I(1)-Ag(3)$^{\#2}$	2.8249(17)	N(1)-C(1)	1.515(12)
I(1)-Ag(1)	2.9017(15)	N(1)-C(26)	1.541(12)
I(2)-Ag(2)	2.7494(15)	C(1)-C(2)	1.498(13)
I(2)-Ag(1)	2.7573(15)	C(2)-C(3)	1.502(13)
I(3)-Ag(3)$^{\#2}$	2.9066(15)	C(3)-C(4)	1.527(15)
I(3)-Ag(3)	2.9241(15)	C(4)-C(5)	1.517(16)
I(3)-Ag(1)	2.9291(16)	C(5)-C(6)	1.534(15)
I(3)-Ag(2)$^{\#3}$	2.9296(15)	C(6)-C(7)	1.488(16)
I(4)-Ag(1)	2.8909(15)	C(7)-C(8)	1.498(16)
I(4)-Ag(2)$^{\#3}$	2.8964(16)	C(8)-C(9)	1.500(17)
I(4)-Ag(4)$^{\#1}$	2.8977(15)	C(9)-C(10)	1.488(16)
I(4)-Ag(4)	2.9003(15)	C(10)-C(11)	1.480(17)
I(5)-Ag(4)$^{\#3}$	2.8252(16)	C(11)-C(12)	1.565(18)
I(5)-Ag(3)$^{\#3}$	2.8336(16)	C(13)-C(14)	1.501(13)
I(5)-Ag(2)	2.8928(15)	C(14)-C(15)	1.522(16)
Ag(2)-I(4)$^{\#3}$	2.8964(16)	C(15)-C(16)	1.566(16)
Ag(2)-I(3)$^{\#3}$	2.9297(15)	C(16)-C(17)	1.467(15)
Ag(3)-I(1)$^{\#2}$	2.8248(17)	C(17)-C(18)	1.507(15)
Ag(3)-I(5)$^{\#3}$	2.8336(16)	C(18)-C(19)	1.482(17)
Ag(3)-I(3)$^{\#2}$	2.9066(15)	C(19)-C(20)	1.491(16)
Ag(4)-I(1)$^{\#1}$	2.8215(16)	C(20)-C(21)	1.506(17)
Ag(4)-I(5)$^{\#3}$	2.8252(16)	C(21)-C(22)	1.491(16)
Ag(4)-I(4)$^{\#1}$	2.8977(15)	C(22)-C(23)	1.516(18)
N(1)-C(13)	1.504(12)	C(23)-C(24)	1.483(18)

Ag(4)$^{\#1}$-I(1)-Ag(3)$^{\#2}$	106.80(5)	Ag(4)$^{\#3}$-I(5)-Ag(3)$^{\#3}$	110.94(5)
Ag(4)$^{\#1}$-I(1)-Ag(1)	70.40(4)	Ag(4)$^{\#3}$-I(5)-Ag(2)	70.98(4)
Ag(3)$^{\#2}$-I(1)-Ag(1)	73.77(4)	Ag(3)$^{\#3}$-I(5)-Ag(2)	78.34(4)
Ag(2)-I(2)-Ag(1)	104.64(5)	I(2)-Ag(1)-I(4)	109.52(4)
Ag(3)$^{\#2}$-I(3)-Ag(3)	65.68(5)	I(2)-Ag(1)-I(1)	105.60(5)
Ag(3)$^{\#2}$-I(3)-Ag(1)	72.18(4)	I(4)-Ag(1)-I(1)	109.01(4)
Ag(3)-I(3)-Ag(1)	110.16(4)	I(2)-Ag(1)-I(3)	115.25(4)
Ag(3)$^{\#2}$-I(3)-Ag(2)$^{\#3}$	108.61(4)	I(4)-Ag(1)-I(3)	111.58(5)
Ag(3)-I(3)-Ag(2)$^{\#3}$	76.33(4)	I(1)-Ag(1)-I(3)	105.48(4)
Ag(1)-I(3)-Ag(2)$^{\#3}$	67.69(4)	I(2)-Ag(2)-I(5)	108.88(5)
Ag(1)-I(4)-Ag(2)$^{\#3}$	68.64(5)	I(2)-Ag(2)-I(4)$^{\#3}$	108.43(4)
Ag(1)-I(4)-Ag(4)$^{\#1}$	69.50(4)	I(5)-Ag(2)-I(4)$^{\#3}$	108.61(4)
Ag(2)$^{\#3}$-I(4)-Ag(4)$^{\#1}$	110.19(4)	I(2)-Ag(2)-I(3)$^{\#3}$	117.29(5)
Ag(1)-I(4)-Ag(4)	108.56(4)	I(5)-Ag(2)-I(3)$^{\#3}$	101.78(4)
Ag(2)$^{\#3}$-I(4)-Ag(4)	69.89(4)	I(4)$^{\#3}$-Ag(2)-I(3)$^{\#3}$	111.41(5)
Ag(4)$^{\#1}$-I(4)-Ag(4)	74.03(5)	I(1)$^{\#2}$-Ag(3)-I(5)$^{\#3}$	105.25(5)

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(Table 3. continued)

I(1)$^{\#2}$-Ag(3)-I(3)$^{\#2}$	108.13(4)	C(5)-C(4)-C(3)	114.0(8)
I(5)$^{\#3}$-Ag(3)-I(3)$^{\#2}$	111.39(5)	C(4)-C(5)-C(6)	113.7(8)
I(1)$^{\#2}$-Ag(3)-I(3)	113.98(5)	C(7)-C(6)-C(5)	117.6(9)
I(5)$^{\#3}$-Ag(3)-I(3)	103.37(4)	C(6)-C(7)-C(8)	116.9(10)
I(3)$^{\#2}$-Ag(3)-I(3)	114.32(5)	C(7)-C(8)-C(9)	116.4(10)
I(1)$^{\#1}$-Ag(4)-I(5)$^{\#3}$	113.35(5)	C(10)-C(9)-C(8)	114.4(10)
I(1)$^{\#1}$-Ag(4)-I(4)$^{\#1}$	111.09(4)	C(11)-C(10)-C(9)	117.4(11)
I(5)$^{\#3}$-Ag(4)-I(4)$^{\#1}$	107.69(4)	C(10)-C(11)-C(12)	117.2(11)
I(1)$^{\#1}$-Ag(4)-I(4)	108.10(4)	C(14)-C(13)-N(1)	115.2(9)
I(5)$^{\#3}$-Ag(4)-I(4)	110.40(4)	C(13)-C(14)-C(15)	112.5(10)
I(4)$^{\#1}$-Ag(4)-I(4)	105.97(5)	C(14)-C(15)-C(16)	112.1(9)
C(13)-N(1)-C(25)	109.4(8)	C(17)-C(16)-C(15)	116.1(10)
C(13)-N(1)-C(1)	113.5(8)	C(16)-C(17)-C(18)	115.5(10)
C(25)-N(1)-C(1)	111.6(7)	C(19)-C(18)-C(17)	115.7(10)
C(13)-N(1)-C(26)	108.4(7)	C(18)-C(19)-C(20)	117.2(10)
C(25)-N(1)-C(26)	106.7(8)	C(19)-C(20)-C(21)	118.2(10)
C(1)-N(1)-C(26)	106.9(8)	C(22)-C(21)-C(20)	117.0(10)
C(2)-C(1)-N(1)	114.3(8)	C(21)-C(22)-C(23)	117.4(11)
C(1)-C(2)-C(3)	111.2(8)	C(24)-C(23)-C(22)	115.8(13)
C(2)-C(3)-C(4)	115.3(9)		

Symmetry transformation codes: #1 (2-*x*, -*y*, 2-*z*); #2 (3-*x*, -*y*, 2-*z*);

#3 (2-*x*, 1-*y*, 2-*z*).