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catena-Poly[[bis[μ-2-(3-pyridyl)-1*H*-benzimidazole]disilver(I)]-μ-benzene-1,4-disulfonato]

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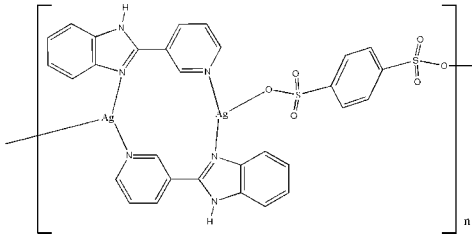
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.008 Å; R factor = 0.061; wR factor = 0.188; data-to-parameter ratio = 15.2.

The title compound, $[Ag_2(C_6H_4O_6S_2)(C_{12}H_9N_3)_2]_n$, is a coordination polymer prepared by a hydrothermal reaction. Two Ag^I atoms are connected by two 2-(3-pyridyl)-benzimidazole ligands, resulting in a binuclear macrocycle. The bridging benzene-1,4-disulfonate ligands link the binuclear units, forming a chain. The crystal packing is stabilized by N—H···O hydrogen bonds.

Related literature

For related structures, see: Yuan *et al.* (2001); Xiong *et al.* (2001); Su *et al.* (1999). For related literature, see: Alcade *et al.* (1992).



Experimental

Crystal data

$[Ag_2(C_6H_4O_6S_2)(C_{12}H_9N_3)_2]$
M_r = 421.20
Triclinic, $P\overline{1}$
a = 7.547 (3) Å
b = 10.060 (4) Å
c = 10.286 (4) Å
α = 77.262 (11)°
β = 69.963 (11)°
γ = 77.409 (10)°
V = 706.9 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.59 mm^{-1}
T = 293 (2) K
0.60 × 0.35 × 0.10 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*CrystalStructure*; Rigaku, 2000)
T_{min} = 0.518, T_{max} = 0.850
5340 measured reflections
3152 independent reflections
2784 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.188
S = 1.11
3152 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.85 e Å^{-3}
$\Delta\rho_{min}$ = −1.86 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3B···O2^{i}	0.86	1.83	2.677 (6)	169

Symmetry code: (i) $-x, -y+1, -z+1$.

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CrystalStructure* (Rigaku, 2000); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2575).

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supplementary materials

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catena-Poly[[bis[μ-2-(3-pyridyl)-1*H*-benzimidazole]disilver(I)]-μ-benzene-1,4-disulfonato]

J. Chen and Y. Ruan

Comment

4-sulfobenzoic acid is an efficient O donor ligand, exhibiting versatile coordination mode and hydrogen bonding interaction in the assembly of metal-organic coordination polymers (Yuan *et al.*, 2001), 4-sulfobenzoic acid could be *in situ* synthesized into benzene-1,4-disulfonate (Xiong *et al.*, 2001). 2-(3-pyridyl)benzimidazole has been reported to connect the Ag^I ions, resulting in a binuclear macrocyclic (Su *et al.*, 1999). Herein, we report the synthesis and structure of the coordination polymer on the basis of bridging benzene-1,4-disulfonate ligands and $[Ag_2(C_{12}H_9N_3)_2]$ binuclear units.

In the title compound, Ag^I exhibits a distorted trigonal planar geometry (Fig. 1). Each two Ag^I atoms are connected with two 2-(3-pyridyl)benzimidazole ligands in the end to end mode *via* N_{py} and N_{BIm} donor atoms, forming a binuclear macrocyclic. The coordination sphere of Ag^I is completed by an oxygen atom from benzene-1,4-disulfonate with bis(monodentate) coordination fashion. The bridging benzene-1,4-disulfonate ligands link the binuclear units, forming a chain (Fig. 2). The chains are assembled into a two-dimensional network by the N—H···O hydrogen bonds as well as π-π interactions between the benzimidazolyl rings of 2-(3-pyridyl)benzimidazole ligands (the perpendicular distance is about 3.43 Å) (Fig. 3). The crystal packing can be viewed as layered arrangement of the two-dimensional supramolecular networks (Fig. 4).

Experimental

A solution of Ag_2O (0.07 g, 0.30 mmol), 2-(3-pyridyl)benzimidazole (Alcade *et al.*, 1992) (0.14 g, 0.61 mmol) 4-sulfobenzoic acid (0.06 g, 0.30 mmol) and H_2O (15 ml) was stirred under ambient condition and then sealed in teflon-lined stainless steel vessel, heated at 403 K for 4 days and cooled to room temperature for 3 days, creating the colorless crystals of the title compound.

Refinement

All H atoms were fixed geometrically and allowed to ride on their attached atoms with C—H=0.93 Å, N—H=0.86 Å and U(H) = 1.2 U_{eq}(C,*N*).

Figures

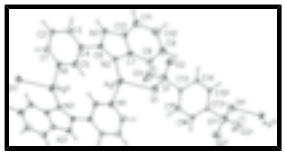

Fig. 1. A view of the molecular structue of the title compound. Displacement ellipsoids are drawn at the 30% probbability level and H atoms are shown as small spheres of arbitrary radii. [Symmetry code: (i)1 − *x*, 1 − *y*, −*z*; (ii)-1 − *x*, 2 − *y*, −*z*.]

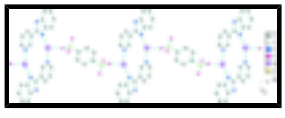

Fig. 2. A view of the one-dimensional chain of the title compound. The hydrogen atoms are omitted for clarity.

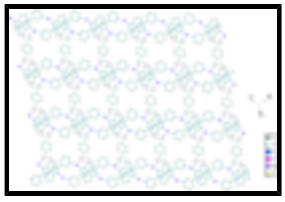

Fig. 3. A view of the two-dimensional sheet of the title compound. The hydrogen atoms are omitted for clarity. Hydrogen bonds are shown as dashed lines.

Fig. 4. The crystal packing of the title compound. The hydrogen atoms are omitted for clarity. Hydrogen bonds are shown as dashed lines.

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Crystal data

$[Ag_2(C_6H_4S_2O_6)(C_{12}H_9N_3)_2]$	$Z = 2$
$M_r = 421.20$	$F_{000} = 418$
Triclinic, $P\bar{1}$	$D_x = 1.979$ Mg m^{-3}
Hall symbol: -p 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.547$ (3) Å	Cell parameters from 2133 reflections
$b = 10.060$ (4) Å	$\theta = 2.9$–27.5º
$c = 10.286$ (4) Å	$\mu = 1.59$ mm^{-1}
$\alpha = 77.262$ (11)º	$T = 293$ (2) K
$\beta = 69.963$ (11)º	Prism, colorless
$\gamma = 77.409$ (10)º	0.60 × 0.35 × 0.10 mm
$V = 706.9$ (5) Å^3	

Data collection

Rigaku Mercury CCD diffractometer	3152 independent reflections
Radiation source: Rotating Anode	2784 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.020$
$T = 293$(2) K	$\theta_{max} = 27.5$º
ω scan	$\theta_{min} = 2.9$º
Absorption correction: multi-scan (CrystalStructure; Rigaku, 2000)	$h = -9 \rightarrow 9$
$T_{min} = 0.518$, $T_{max} = 0.850$	$k = -13 \rightarrow 13$
5340 measured reflections	$l = -8 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.061$	H-atom parameters constrained
$wR(F^2) = 0.188$	$w = 1/[\sigma^2(F_o^2) + (0.1114P)^2 + 1.6836P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.11$	$(\Delta/\sigma)_{max} < 0.001$
3152 reflections	$\Delta\rho_{max} = 0.85$ e Å^{-3}
208 parameters	$\Delta\rho_{min} = -1.86$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ag1	0.21136 (7)	0.66405 (5)	0.12969 (4)	0.0504 (2)
S1	−0.2367 (3)	0.7926 (2)	0.1437 (2)	0.0657 (5)
C1	0.7242 (8)	0.1820 (6)	0.1720 (6)	0.0411 (12)
H1A	0.8100	0.1153	0.1224	0.049*
C2	0.6483 (9)	0.1494 (6)	0.3124 (7)	0.0450 (13)
H2A	0.6849	0.0623	0.3579	0.054*
C3	0.5173 (8)	0.2445 (6)	0.3881 (6)	0.0406 (12)
H3A	0.4635	0.2218	0.4845	0.049*
C4	0.4660 (7)	0.3754 (5)	0.3187 (5)	0.0288 (9)
C5	0.5556 (8)	0.4020 (6)	0.1745 (6)	0.0378 (11)
H5A	0.5274	0.4899	0.1269	0.045*
C6	0.3252 (7)	0.4808 (5)	0.3941 (5)	0.0283 (9)
C7	0.1248 (7)	0.6644 (5)	0.4484 (5)	0.0304 (9)
C8	0.0034 (8)	0.7919 (6)	0.4505 (6)	0.0393 (12)
H8A	−0.0086	0.8474	0.3678	0.047*
C9	−0.0988 (9)	0.8330 (6)	0.5804 (7)	0.0446 (13)
H9A	−0.1781	0.9178	0.5850	0.054*
C10	−0.0815 (10)	0.7451 (7)	0.7058 (7)	0.0476 (14)
H10A	−0.1530	0.7730	0.7915	0.057*
C11	0.0369 (8)	0.6208 (6)	0.7045 (6)	0.0394 (11)
H11A	0.0479	0.5646	0.7871	0.047*
C12	0.1399 (7)	0.5822 (5)	0.5741 (5)	0.0306 (10)
C13	−0.3807 (7)	0.9099 (5)	0.0677 (6)	0.0321 (10)
C14	−0.5786 (7)	0.9207 (5)	0.1275 (5)	0.0346 (10)
H14A	−0.6305	0.8677	0.2134	0.042*
C15	−0.3035 (7)	0.9905 (5)	−0.0596 (6)	0.0357 (11)

H15A	−0.1718	0.9843	−0.0990	0.043*
N1	0.6796 (7)	0.3085 (5)	0.1011 (5)	0.0400 (10)
N2	0.2393 (6)	0.5984 (4)	0.3372 (4)	0.0307 (8)
N3	0.2692 (6)	0.4672 (4)	0.5352 (4)	0.0327 (9)
H3B	0.3074	0.3988	0.5909	0.039*
O1	−0.0735 (7)	0.8405 (6)	0.1194 (6)	0.0690 (16)
O2	−0.3410 (9)	0.7512 (7)	0.2775 (6)	0.087 (2)
O3	−0.179 (3)	0.6689 (9)	0.0723 (15)	0.173 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0630 (4)	0.0477 (3)	0.0345 (3)	0.0168 (2)	−0.0243 (2)	−0.0043 (2)
S1	0.0677 (12)	0.0610 (11)	0.0589 (11)	0.0008 (9)	−0.0245 (9)	0.0067 (9)
C1	0.043 (3)	0.035 (3)	0.046 (3)	0.007 (2)	−0.023 (2)	−0.008 (2)
C2	0.051 (3)	0.025 (2)	0.051 (3)	0.002 (2)	−0.016 (3)	0.003 (2)
C3	0.040 (3)	0.032 (2)	0.039 (3)	−0.001 (2)	−0.009 (2)	0.006 (2)
C4	0.028 (2)	0.025 (2)	0.033 (2)	−0.0015 (17)	−0.0134 (18)	0.0005 (18)
C5	0.043 (3)	0.033 (3)	0.032 (3)	0.010 (2)	−0.016 (2)	−0.003 (2)
C6	0.031 (2)	0.027 (2)	0.026 (2)	−0.0049 (18)	−0.0126 (18)	0.0012 (17)
C7	0.030 (2)	0.028 (2)	0.033 (2)	−0.0055 (18)	−0.0107 (18)	−0.0022 (18)
C8	0.042 (3)	0.028 (2)	0.044 (3)	0.000 (2)	−0.014 (2)	−0.003 (2)
C9	0.051 (3)	0.037 (3)	0.047 (3)	−0.005 (2)	−0.014 (3)	−0.012 (2)
C10	0.056 (4)	0.048 (3)	0.040 (3)	−0.011 (3)	−0.007 (3)	−0.019 (3)
C11	0.044 (3)	0.044 (3)	0.031 (3)	−0.011 (2)	−0.010 (2)	−0.006 (2)
C12	0.034 (2)	0.029 (2)	0.031 (2)	−0.0069 (18)	−0.0118 (19)	−0.0027 (18)
C13	0.033 (2)	0.022 (2)	0.037 (3)	0.0004 (18)	−0.010 (2)	−0.0032 (18)
C14	0.035 (2)	0.031 (2)	0.029 (2)	−0.0045 (19)	−0.0035 (19)	0.0011 (19)
C15	0.025 (2)	0.036 (2)	0.039 (3)	−0.0014 (19)	−0.0043 (19)	−0.004 (2)
N1	0.042 (2)	0.039 (2)	0.034 (2)	0.0123 (19)	−0.0174 (19)	−0.0069 (18)
N2	0.033 (2)	0.0275 (19)	0.029 (2)	−0.0023 (16)	−0.0105 (16)	−0.0005 (15)
N3	0.039 (2)	0.028 (2)	0.030 (2)	−0.0018 (17)	−0.0138 (17)	0.0006 (16)
O1	0.036 (2)	0.087 (4)	0.070 (3)	0.006 (2)	−0.026 (2)	0.016 (3)
O2	0.069 (3)	0.105 (5)	0.058 (3)	−0.004 (3)	−0.030 (3)	0.050 (3)
O3	0.280 (16)	0.066 (5)	0.213 (12)	0.038 (7)	−0.158 (12)	−0.039 (6)

Geometric parameters (Å, °)

Ag1—N2	2.159 (4)	C7—N2	1.379 (7)
Ag1—N1^{i}	2.205 (5)	C7—C8	1.404 (7)
Ag1—O1	2.489 (5)	C7—C12	1.399 (7)
S1—O1	1.344 (6)	C8—C9	1.396 (8)
S1—O2	1.355 (6)	C8—H8A	0.9300
S1—O3	1.491 (10)	C9—C10	1.422 (9)
S1—C13	1.674 (5)	C9—H9A	0.9300
C1—C2	1.352 (9)	C10—C11	1.369 (9)
C1—N1	1.355 (7)	C10—H10A	0.9300
C1—H1A	0.9300	C11—C12	1.391 (7)

C2—C3	1.374 (8)	C11—H11A	0.9300
C2—H2A	0.9300	C12—N3	1.377 (7)
C3—C4	1.396 (7)	C13—C15	1.388 (7)
C3—H3A	0.9300	C13—C14	1.396 (7)
C4—C5	1.395 (7)	C14—C15^{ii}	1.371 (8)
C4—C6	1.471 (7)	C14—H14A	0.9300
C5—N1	1.333 (7)	C15—C14^{ii}	1.371 (8)
C5—H5A	0.9300	C15—H15A	0.9300
C6—N2	1.335 (6)	N3—O2^{iii}	2.677 (6)
C6—N3	1.349 (6)	N3—H3B	0.8600
N2—Ag1—N1^{i}	153.94 (18)	C8—C9—C10	120.0 (6)
N2—Ag1—O1	114.05 (18)	C8—C9—H9A	120.0
N1^{i}—Ag1—O1	90.56 (18)	C10—C9—H9A	120.0
O1—S1—O2	119.3 (4)	C11—C10—C9	122.2 (6)
O1—S1—O3	105.1 (8)	C11—C10—H10A	118.9
O2—S1—O3	106.4 (7)	C9—C10—H10A	118.9
O1—S1—C13	109.6 (3)	C10—C11—C12	117.1 (5)
O2—S1—C13	107.7 (3)	C10—C11—H11A	121.5
O3—S1—C13	108.3 (5)	C12—C11—H11A	121.5
C2—C1—N1	122.3 (5)	N3—C12—C11	132.2 (5)
C2—C1—H1A	118.9	N3—C12—C7	105.2 (4)
N1—C1—H1A	118.9	C11—C12—C7	122.6 (5)
C1—C2—C3	120.2 (5)	C15—C13—C14	119.9 (5)
C1—C2—H2A	119.9	C15—C13—S1	119.9 (4)
C3—C2—H2A	119.9	C14—C13—S1	120.1 (4)
C2—C3—C4	119.2 (5)	C15^{ii}—C14—C13	120.0 (5)
C2—C3—H3A	120.4	C15^{ii}—C14—H14A	120.0
C4—C3—H3A	120.4	C13—C14—H14A	120.0
C3—C4—C5	116.9 (5)	C14^{ii}—C15—C13	120.1 (5)
C3—C4—C6	121.6 (5)	C14^{ii}—C15—H15A	120.0
C5—C4—C6	121.5 (4)	C13—C15—H15A	120.0
N1—C5—C4	123.6 (5)	C5—N1—C1	117.8 (5)
N1—C5—H5A	118.2	C5—N1—Ag1^{i}	124.4 (4)
C4—C5—H5A	118.2	C1—N1—Ag1^{i}	117.3 (4)
N2—C6—N3	111.8 (4)	C6—N2—C7	105.5 (4)
N2—C6—C4	126.7 (4)	C6—N2—Ag1	131.1 (4)
N3—C6—C4	121.6 (4)	C7—N2—Ag1	121.9 (3)
N2—C7—C8	130.4 (5)	C6—N3—C12	108.0 (4)
N2—C7—C12	109.6 (4)	C6—N3—O2^{iii}	129.2 (4)
C8—C7—C12	120.0 (5)	C12—N3—O2^{iii}	122.3 (4)
C7—C8—C9	118.0 (5)	C6—N3—H3B	126.0
C7—C8—H8A	121.0	C12—N3—H3B	126.0
C9—C8—H8A	121.0	S1—O1—Ag1	116.3 (4)
N1—C1—C2—C3	1.8 (10)	S1—C13—C15—C14^{ii}	175.0 (4)
C1—C2—C3—C4	−0.9 (9)	C4—C5—N1—C1	−1.9 (9)

C2—C3—C4—C5	−1.1 (8)	C4—C5—N1—Ag1^{i}	169.8 (4)
C2—C3—C4—C6	179.4 (5)	C2—C1—N1—C5	−0.4 (9)
C3—C4—C5—N1	2.6 (8)	C2—C1—N1—Ag1^{i}	−172.7 (5)
C6—C4—C5—N1	−177.9 (5)	N3—C6—N2—C7	1.2 (5)
C3—C4—C6—N2	−166.6 (5)	C4—C6—N2—C7	−178.3 (4)
C5—C4—C6—N2	14.0 (8)	N3—C6—N2—Ag1	−164.2 (3)
C3—C4—C6—N3	14.0 (7)	C4—C6—N2—Ag1	16.3 (7)
C5—C4—C6—N3	−165.5 (5)	C8—C7—N2—C6	179.5 (5)
N2—C7—C8—C9	179.2 (5)	C12—C7—N2—C6	−1.5 (5)
C12—C7—C8—C9	0.4 (8)	C8—C7—N2—Ag1	−13.4 (7)
C7—C8—C9—C10	−1.4 (9)	C12—C7—N2—Ag1	165.5 (3)
C8—C9—C10—C11	1.6 (9)	N1^{i}—Ag1—N2—C6	−46.3 (6)
C9—C10—C11—C12	−0.6 (9)	O1—Ag1—N2—C6	154.2 (4)
C10—C11—C12—N3	179.8 (5)	N1^{i}—Ag1—N2—C7	150.3 (4)
C10—C11—C12—C7	−0.5 (8)	O1—Ag1—N2—C7	−9.2 (4)
N2—C7—C12—N3	1.3 (5)	N2—C6—N3—C12	−0.4 (5)
C8—C7—C12—N3	−179.6 (4)	C4—C6—N3—C12	179.1 (4)
N2—C7—C12—C11	−178.5 (5)	N2—C6—N3—O2^{iii}	171.1 (4)
C8—C7—C12—C11	0.6 (7)	C4—C6—N3—O2^{iii}	−9.3 (7)
O1—S1—C13—C15	35.5 (6)	C11—C12—N3—C6	179.2 (5)
O2—S1—C13—C15	166.7 (6)	C7—C12—N3—C6	−0.6 (5)
O3—S1—C13—C15	−78.7 (9)	C11—C12—N3—O2^{iii}	6.9 (8)
O1—S1—C13—C14	−148.6 (5)	C7—C12—N3—O2^{iii}	−172.8 (3)
O2—S1—C13—C14	−17.4 (7)	O2—S1—O1—Ag1	79.7 (5)
O3—S1—C13—C14	97.2 (9)	O3—S1—O1—Ag1	−39.4 (6)
C15—C13—C14—C15^{ii}	0.8 (9)	C13—S1—O1—Ag1	−155.6 (3)
S1—C13—C14—C15^{ii}	−175.0 (4)	N2—Ag1—O1—S1	−86.9 (4)
C14—C13—C15—C14^{ii}	−0.8 (9)	N1^{i}—Ag1—O1—S1	101.9 (4)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*; (ii) −*x*−1, −*y*+2, −*z*; (iii) −*x*, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3B···O2^{iii}	0.86	1.83	2.677 (6)	169

Symmetry codes: (iii) −*x*, −*y*+1, −*z*+1.

Fig. 1

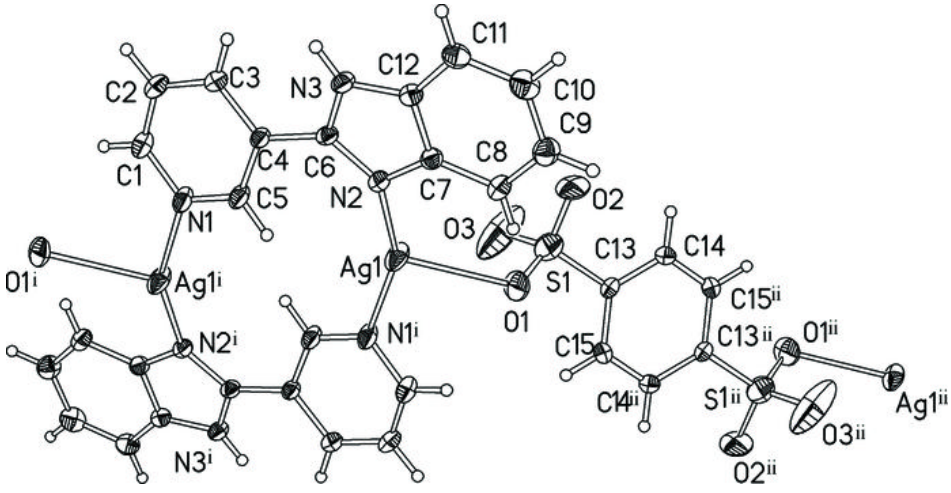
C11
C12
N3
C3
C2
C10
C9
C8
C4
C6
C7
C1
C5
N2
O2
O3
N1
C13
C14
O1i
Ag1i
Ag1
S1
C15ii
O1
C13ii
O1ii
N2i
N1i
C15
C14ii
S1ii
Ag1ii
O3ii
N3i
O2ii

Fig. 2

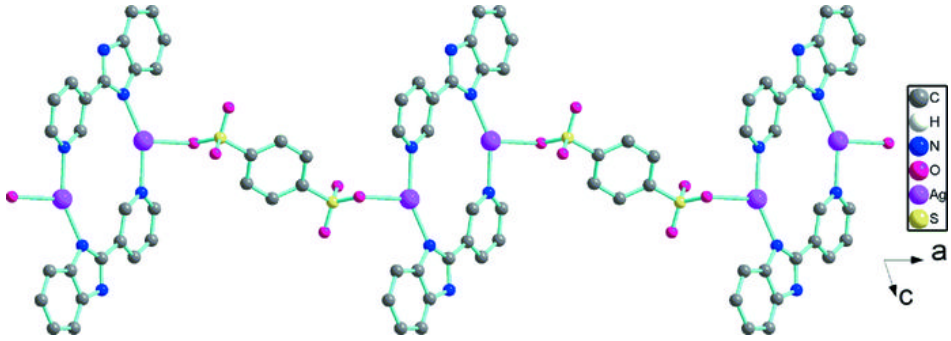

Fig. 3

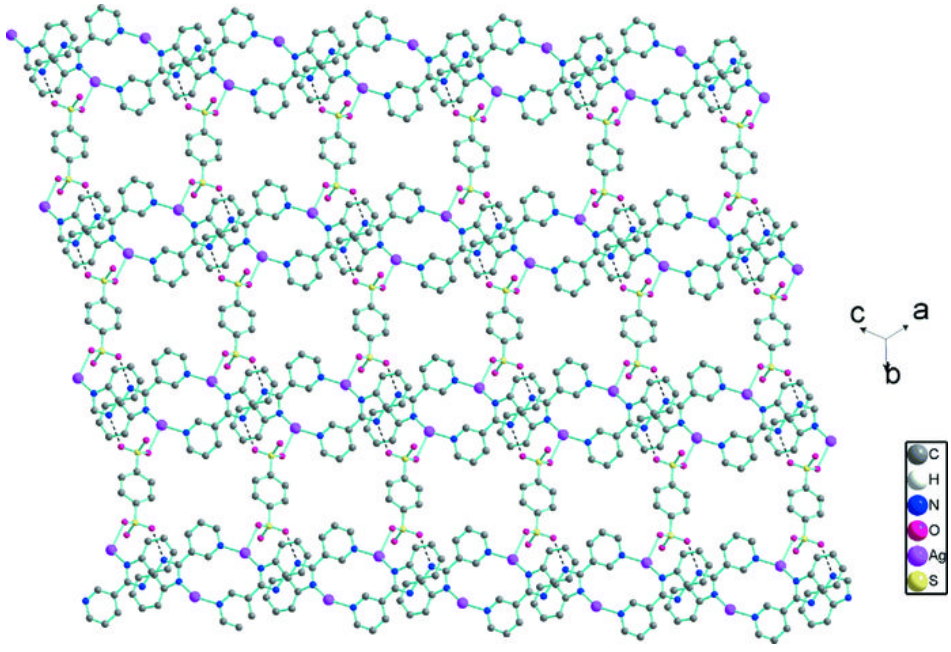

Fig. 4