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catena-Poly[silver(I)-μ-4-aminobenzenesulfonato-μ-2,3-diethylpyrazine]

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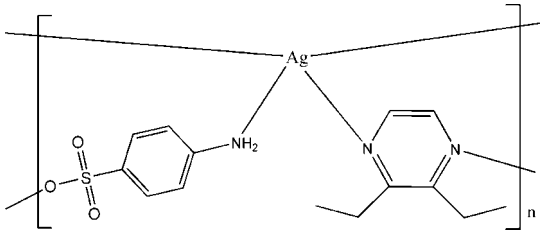
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.034; wR factor = 0.079; data-to-parameter ratio = 16.6.

In the title compound, $[Ag(C_6H_6NO_3S)(C_8H_8N_2)]$, the Ag^I cation is four-coordinated by three N atoms from two different 2,3-diethylpyrazine ligands and one $-NH_2$ group of a 4-aminobenzenesulfonate ligand, and one sulfonate O atom in a distorted tetrahedral coordination geometry. The Ag^I centers are doubly bridged by both types of ligands, forming a one-dimensional chain. N—H···O hydrogen bonds complete the structure.

Related literature

For studies on silver sulfonates, see Liu *et al.*, (2007). For related literature, see: Cote & Shimizu (2003).



Experimental

Crystal data

$[Ag(C_6H_6NO_3S)(C_8H_8N_2)]$
M_r = 416.24
Orthorhombic, $Pca2_1$
a = 8.6095 (17) Å
b = 12.322 (3) Å
c = 14.342 (3) Å
V = 1521.5 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.48 mm^{-1}
T = 293 (2) K
0.31 × 0.22 × 0.17 mm

Data collection

Rigaku R-AXIS RAPID CCD diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.626, T_{max} = 0.779
13887 measured reflections
3443 independent reflections
2756 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.079
S = 1.05
3443 reflections
207 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.68 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}
Absolute structure: Flack (1983), with 1630 Friedel pairs
Flack parameter: 0.02 (4)

Table 1
Selected bond lengths (Å).

Ag1—N2	2.287 (4)	Ag1—N1^{i}	2.372 (4)
Ag1—N3	2.367 (4)	Ag1—O3^{ii}	2.451 (3)

Symmetry codes: (i) $-x+\frac{3}{2}, y, z+\frac{1}{2}$; (ii) $-x+\frac{3}{2}, y, z-\frac{1}{2}$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N3—HN2···O2^{iii}	0.85 (3)	2.16 (3)	2.923 (6)	149 (5)
N3—HN1···O2^{iv}	0.86 (3)	2.27 (3)	3.042 (5)	150 (4)

Symmetry codes: (iii) $-x+1, -y+1, z-\frac{1}{2}$; (iv) $-x+\frac{1}{2}, y, z-\frac{1}{2}$.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); 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: BG2112).

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supplementary materials

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catena-Poly[silver(I)-μ-4-aminobenzenesulfonato-μ-2,3-diethylpyrazine]

H.-Y. Liu, J.-C. Ma and J. Yang

Comment

Silver(I) sulfonate coordination polymers have received much attention for their interesting structural features and potential application (Cote & Shimizu, 2003). Recently, silver(I) sulfonate compounds with nitrogen-based secondary ligands have been studied (Liu *et al.*, 2007). Herein, we present a new sulfonate coordination polymer, namely [Ag(dep)(*L*)] (I), where dep = 2,3-diethylpyrazine and HL= 4-aminobenzenesulfonic acid. To our knowledge, this is the first complex reported which contains dep as a ligand.

Selected parameters are listed in Table 1. The Ag^I cation is four-coordinated by three N atoms from two different dep ligands and one $–NH_2$ group of *L*, and one sulfonate O atom in a distorted tetrahedral coordination geometry (Fig. 1). The Ag—N distances in (I) are similar to those in related compounds (Liu *et al.*, 2007). The Ag^I centers are doubly bridged by both types of ligands to form a one-dimensional chain (Fig. 2). Finally, N—H···O hydrogen bonds complete the structure of (I) (Table 2).

Experimental

An aqueous solution (16 ml) of 4-aminobenzenesulfonic acid (1 mmol) was added to solid Ag_2CO_3 (0.5 mmol) and stirred for several minutes until no further CO_2 was given off. The 2,3-diethylpyrazine (1 mmol) was then added and a precipitate was formed. The precipitate was dissolved by ammonium hydroxide. Crystals of (I) were obtained by evaporation of the solution for one week at room temperature.

Refinement

H atoms of C atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding, with U_{iso}(H)=1.2U_{eq}(carrier). H atoms bonded to N atom were located in a difference map and refined freely, and with U_{iso}(H) = 1.2U_{eq}(N).

Figures

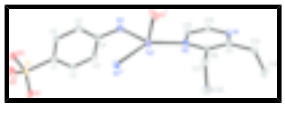

Fig. 1. The structure of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Symmetry code: (i) 1.5 − *x*, *y*, *z* − 1/2; (ii) 1.5 − *x*, *y*, *z* + 1/2.

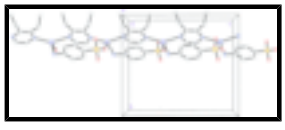

Fig. 2. View of the chain structure of (I).

catena-Poly[silver(I)-μ-4-aminobenzenesulfonato-μ-2,3-diethylpyrazine]

Crystal data

$[Ag(C_6H_6NO_3S)(C_8H_8N_2)]$	F_{000} = 840
M_r = 416.24	D_x = 1.817 Mg m^{-3}
Orthorhombic, $Pca2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2c -2ac	Cell parameters from 11246 reflections
a = 8.6095 (17) Å	θ = 3.0–27.5º
b = 12.322 (3) Å	μ = 1.48 mm^{-1}
c = 14.342 (3) Å	T = 293 (2) K
V = 1521.5 (5) Å^3	Block, colourless
Z = 4	0.31 × 0.22 × 0.17 mm

Data collection

Rigaku R-AXIS RAPID CCD diffractometer	3443 independent reflections
Radiation source: rotating anode	2756 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.040
Detector resolution: 10.0 pixels mm^{-1}	θ_{max} = 27.5º
T = 293(2) K	θ_{min} = 3.2º
ω scans	h = −11→11
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	k = −15→15
T_{min} = 0.626, T_{max} = 0.779	l = −18→18
13887 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.034	$w = 1/[\sigma^2(F_o^2) + (0.0361P)^2 + 0.2752P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.079	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.05	$\Delta\rho_{max}$ = 0.68 e Å^{-3}
3443 reflections	$\Delta\rho_{min}$ = −0.31 e Å^{-3}
207 parameters	Extinction correction: none
3 restraints	Absolute structure: Flack (1983)
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.02 (4)
Secondary atom site location: difference Fourier map	

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	0.75241 (4)	0.26431 (3)	0.84998 (7)	0.04695 (10)
N2	0.7161 (4)	0.2166 (3)	0.6974 (3)	0.0320 (8)
N3	0.5572 (4)	0.3870 (4)	0.8990 (2)	0.0418 (9)
C2	0.3331 (4)	0.3028 (3)	1.1066 (3)	0.0314 (7)
H2	0.2491	0.2583	1.1208	0.038*
C1	0.4096 (4)	0.3569 (4)	1.1770 (2)	0.0309 (9)
C5	0.5817 (5)	0.4358 (4)	1.0639 (3)	0.0370 (10)
H5	0.6650	0.4808	1.0493	0.044*
C4	0.5046 (4)	0.3807 (3)	0.9936 (3)	0.0329 (8)
C3	0.3805 (4)	0.3143 (4)	1.0149 (3)	0.0335 (10)
H3	0.3287	0.2773	0.9677	0.040*
C15	0.6074 (5)	0.2709 (4)	0.6484 (3)	0.0379 (12)
H15	0.5352	0.3134	0.6800	0.046*
C16	0.8158 (4)	0.1530 (4)	0.6489 (3)	0.0297 (9)
C17	0.9340 (5)	0.0913 (4)	0.7056 (3)	0.0369 (10)
H17A	1.0324	0.0920	0.6727	0.044*
H17B	0.9489	0.1284	0.7646	0.044*
C18	0.8893 (6)	−0.0230 (5)	0.7244 (4)	0.0603 (15)
H18A	0.9691	−0.0576	0.7606	0.090*
H18B	0.8766	−0.0609	0.6664	0.090*
H18C	0.7933	−0.0245	0.7584	0.090*
C6	0.5349 (5)	0.4242 (4)	1.1560 (3)	0.0360 (10)
H6	0.5868	0.4610	1.2032	0.043*
O2	0.2572 (3)	0.4407 (3)	1.3140 (2)	0.0509 (8)
O3	0.4825 (3)	0.3370 (3)	1.3513 (2)	0.0602 (9)
O1	0.2466 (4)	0.2486 (3)	1.2958 (3)	0.0693 (14)
S1	0.34471 (10)	0.34335 (8)	1.29348 (7)	0.0329 (2)
C10	0.6010 (5)	0.2649 (4)	0.5534 (3)	0.0349 (11)
H10	0.5247	0.3036	0.5217	0.042*
N1	0.7017 (4)	0.2050 (4)	0.5049 (3)	0.0334 (8)
C11	0.8082 (5)	0.1482 (4)	0.5518 (3)	0.0325 (10)
C12	0.9145 (5)	0.0780 (4)	0.4936 (3)	0.0429 (11)
H12A	1.0060	0.0605	0.5301	0.051*

H12B	0.9483	0.1193	0.4397	0.051*
C13	0.8404 (7)	−0.0264 (5)	0.4606 (4)	0.0612 (15)
H13A	0.9143	−0.0670	0.4246	0.092*
H13B	0.7516	−0.0098	0.4227	0.092*
H13C	0.8084	−0.0684	0.5135	0.092*
HN1	0.475 (3)	0.378 (4)	0.866 (3)	0.054 (15)*
HN2	0.605 (5)	0.447 (2)	0.895 (4)	0.064 (17)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.04408 (15)	0.0751 (2)	0.02168 (13)	−0.00020 (18)	0.00003 (12)	−0.0028 (3)
N2	0.0346 (16)	0.039 (2)	0.0222 (18)	0.0021 (16)	−0.0005 (16)	0.0016 (16)
N3	0.040 (2)	0.058 (3)	0.0277 (17)	0.0066 (18)	0.0032 (16)	0.0097 (17)
C2	0.0300 (16)	0.0350 (19)	0.0292 (18)	−0.0006 (13)	0.000 (2)	0.0033 (19)
C1	0.0307 (18)	0.038 (3)	0.0240 (17)	0.0030 (16)	0.0004 (14)	−0.0017 (17)
C5	0.035 (2)	0.033 (3)	0.043 (2)	−0.0019 (18)	0.0019 (19)	0.0040 (18)
C4	0.0346 (19)	0.037 (2)	0.0274 (17)	0.0097 (17)	0.0035 (16)	0.0046 (17)
C3	0.0314 (19)	0.042 (3)	0.027 (2)	0.0023 (17)	−0.0059 (16)	−0.0020 (18)
C15	0.032 (2)	0.051 (4)	0.030 (2)	0.009 (2)	0.001 (2)	−0.004 (2)
C16	0.028 (2)	0.035 (3)	0.0264 (19)	0.0024 (19)	−0.0020 (17)	−0.0008 (18)
C17	0.035 (2)	0.039 (3)	0.037 (2)	0.0042 (18)	−0.0093 (19)	0.0038 (19)
C18	0.070 (3)	0.044 (3)	0.067 (3)	0.000 (3)	−0.022 (3)	0.017 (3)
C6	0.039 (2)	0.036 (3)	0.034 (2)	0.0005 (18)	−0.0047 (18)	−0.0021 (18)
O2	0.0565 (18)	0.057 (2)	0.0394 (16)	0.0259 (15)	0.0059 (13)	−0.0043 (14)
O3	0.0433 (15)	0.109 (3)	0.0280 (14)	0.0254 (17)	−0.0057 (14)	0.007 (2)
O1	0.109 (4)	0.060 (3)	0.039 (2)	−0.040 (2)	0.027 (2)	−0.0145 (15)
S1	0.0359 (4)	0.0391 (5)	0.0235 (4)	0.0027 (4)	−0.0001 (4)	−0.0027 (4)
C10	0.032 (2)	0.041 (3)	0.032 (2)	0.008 (2)	−0.0043 (18)	0.0017 (19)
N1	0.0310 (16)	0.044 (2)	0.0247 (19)	−0.0011 (18)	0.0029 (17)	0.0011 (17)
C11	0.031 (2)	0.036 (3)	0.031 (2)	−0.003 (2)	0.0013 (17)	0.0013 (18)
C12	0.034 (2)	0.056 (3)	0.039 (2)	0.003 (2)	0.0070 (19)	−0.007 (2)
C13	0.060 (3)	0.064 (4)	0.060 (3)	−0.005 (3)	0.011 (3)	−0.028 (3)

Geometric parameters (Å, °)

Ag1—N2	2.287 (4)	C17—C18	1.486 (7)
Ag1—N3	2.367 (4)	C17—H17A	0.9700
Ag1—N1^{i}	2.372 (4)	C17—H17B	0.9700
Ag1—O3^{ii}	2.451 (3)	C18—H18A	0.9600
N2—C15	1.348 (6)	C18—H18B	0.9600
N2—C16	1.355 (6)	C18—H18C	0.9600
N3—C4	1.432 (5)	C6—H6	0.9300
N3—HN1	0.86 (3)	O2—S1	1.446 (3)
N3—HN2	0.85 (3)	O3—S1	1.450 (3)
C2—C1	1.378 (5)	O3—Ag1^{i}	2.451 (3)
C2—C3	1.384 (6)	O1—S1	1.441 (3)
C2—H2	0.9300	C10—N1	1.334 (6)

C1—C6	1.393 (6)	C10—H10	0.9300
C1—S1	1.769 (4)	N1—C11	1.335 (6)
C5—C4	1.385 (6)	N1—Ag1^{ii}	2.372 (4)
C5—C6	1.388 (6)	C11—C12	1.510 (6)
C5—H5	0.9300	C12—C13	1.512 (7)
C4—C3	1.380 (6)	C12—H12A	0.9700
C3—H3	0.9300	C12—H12B	0.9700
C15—C10	1.367 (5)	C13—H13A	0.9600
C15—H15	0.9300	C13—H13B	0.9600
C16—C11	1.395 (4)	C13—H13C	0.9600
C16—C17	1.508 (6)		
N2—Ag1—N3	110.54 (13)	C16—C17—H17B	108.8
N2—Ag1—N1^{i}	147.11 (11)	H17A—C17—H17B	107.7
N3—Ag1—N1^{i}	92.12 (13)	C17—C18—H18A	109.5
N2—Ag1—O3^{ii}	103.22 (13)	C17—C18—H18B	109.5
N3—Ag1—O3^{ii}	115.15 (14)	H18A—C18—H18B	109.5
N1^{i}—Ag1—O3^{ii}	87.14 (12)	C17—C18—H18C	109.5
C15—N2—C16	117.3 (4)	H18A—C18—H18C	109.5
C15—N2—Ag1	117.8 (3)	H18B—C18—H18C	109.5
C16—N2—Ag1	123.6 (3)	C5—C6—C1	119.5 (4)
C4—N3—Ag1	118.1 (3)	C5—C6—H6	120.2
C4—N3—HN1	104 (3)	C1—C6—H6	120.2
Ag1—N3—HN1	110 (3)	S1—O3—Ag1^{i}	141.0 (2)
C4—N3—HN2	105 (4)	O1—S1—O2	111.2 (2)
Ag1—N3—HN2	101 (4)	O1—S1—O3	115.0 (3)
HN1—N3—HN2	118 (5)	O2—S1—O3	110.8 (2)
C1—C2—C3	120.4 (4)	O1—S1—C1	106.5 (2)
C1—C2—H2	119.8	O2—S1—C1	106.1 (2)
C3—C2—H2	119.8	O3—S1—C1	106.67 (18)
C2—C1—C6	119.9 (3)	N1—C10—C15	121.6 (5)
C2—C1—S1	119.7 (3)	N1—C10—H10	119.2
C6—C1—S1	120.4 (3)	C15—C10—H10	119.2
C4—C5—C6	120.2 (4)	C10—N1—C11	118.3 (4)
C4—C5—H5	119.9	C10—N1—Ag1^{ii}	115.2 (3)
C6—C5—H5	119.9	C11—N1—Ag1^{ii}	121.2 (3)
C3—C4—C5	120.0 (4)	N1—C11—C16	120.8 (5)
C3—C4—N3	119.2 (4)	N1—C11—C12	116.0 (4)
C5—C4—N3	120.7 (4)	C16—C11—C12	123.2 (5)
C4—C3—C2	120.0 (4)	C11—C12—C13	113.8 (4)
C4—C3—H3	120.0	C11—C12—H12A	108.8
C2—C3—H3	120.0	C13—C12—H12A	108.8
N2—C15—C10	121.4 (5)	C11—C12—H12B	108.8
N2—C15—H15	119.3	C13—C12—H12B	108.8
C10—C15—H15	119.3	H12A—C12—H12B	107.7
N2—C16—C11	120.5 (5)	C12—C13—H13A	109.5
N2—C16—C17	116.2 (3)	C12—C13—H13B	109.5
C11—C16—C17	123.3 (5)	H13A—C13—H13B	109.5

C18—C17—C16	113.7 (4)	C12—C13—H13C	109.5
C18—C17—H17A	108.8	H13A—C13—H13C	109.5
C16—C17—H17A	108.8	H13B—C13—H13C	109.5
C18—C17—H17B	108.8		
N3—Ag1—N2—C15	8.8 (4)	C4—C5—C6—C1	−0.2 (7)
N1^{i}—Ag1—N2—C15	139.5 (3)	C2—C1—C6—C5	−0.1 (7)
O3^{ii}—Ag1—N2—C15	−114.9 (3)	S1—C1—C6—C5	−178.4 (4)
N3—Ag1—N2—C16	175.5 (4)	Ag1^{i}—O3—S1—O1	82.1 (4)
N1^{i}—Ag1—N2—C16	−53.8 (5)	Ag1^{i}—O3—S1—O2	−150.8 (3)
O3^{ii}—Ag1—N2—C16	51.8 (4)	Ag1^{i}—O3—S1—C1	−35.7 (4)
N2—Ag1—N3—C4	145.8 (3)	C2—C1—S1—O1	17.3 (4)
N1^{i}—Ag1—N3—C4	−9.9 (3)	C6—C1—S1—O1	−164.4 (4)
O3^{ii}—Ag1—N3—C4	−97.7 (3)	C2—C1—S1—O2	−101.3 (4)
C3—C2—C1—C6	0.4 (6)	C6—C1—S1—O2	77.0 (4)
C3—C2—C1—S1	178.7 (3)	C2—C1—S1—O3	140.5 (3)
C6—C5—C4—C3	0.3 (7)	C6—C1—S1—O3	−41.2 (4)
C6—C5—C4—N3	−176.3 (4)	N2—C15—C10—N1	0.1 (9)
Ag1—N3—C4—C3	−90.5 (4)	C15—C10—N1—C11	1.5 (8)
Ag1—N3—C4—C5	86.1 (5)	C15—C10—N1—Ag1^{ii}	−153.2 (5)
C5—C4—C3—C2	0.0 (6)	C10—N1—C11—C16	−1.2 (8)
N3—C4—C3—C2	176.7 (4)	Ag1^{ii}—N1—C11—C16	151.9 (4)
C1—C2—C3—C4	−0.3 (6)	C10—N1—C11—C12	177.5 (4)
C16—N2—C15—C10	−2.1 (8)	Ag1^{ii}—N1—C11—C12	−29.4 (6)
Ag1—N2—C15—C10	165.5 (5)	N2—C16—C11—N1	−0.7 (9)
C15—N2—C16—C11	2.3 (8)	C17—C16—C11—N1	−179.6 (4)
Ag1—N2—C16—C11	−164.4 (4)	N2—C16—C11—C12	−179.3 (4)
C15—N2—C16—C17	−178.7 (4)	C17—C16—C11—C12	1.9 (9)
Ag1—N2—C16—C17	14.5 (6)	N1—C11—C12—C13	−77.5 (6)
N2—C16—C17—C18	98.0 (5)	C16—C11—C12—C13	101.2 (6)
C11—C16—C17—C18	−83.1 (6)		

Symmetry codes: (i) −*x*+3/2, *y*, *z*+1/2; (ii) −*x*+3/2, *y*, *z*−1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—HN2···O2^{iii}	0.85 (3)	2.16 (3)	2.923 (6)	149 (5)
N3—HN1···O2^{iv}	0.86 (3)	2.27 (3)	3.042 (5)	150 (4)

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

Fig. 1

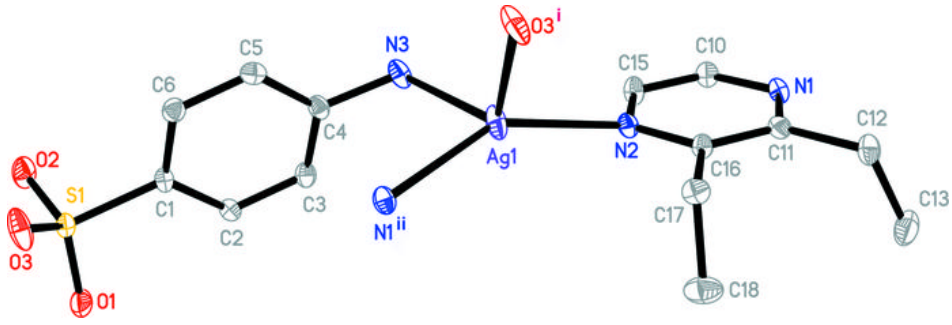
O3 i
N3
C5
C6
C4
C15
C10
N1
C12
O2
S1
C1
C3
Ag1
N2
C16
C11
C13
C2
N1 ii
C17
O3
O1
C18

Fig. 2