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Bis[μ -*N*-(pyridin-2-yl)methanesulfonamido- κ^2 *N*:*N'*]*silver*(I)Hui-Ling Hu^{a,b} and Chun-Wei Yeh^{b*}

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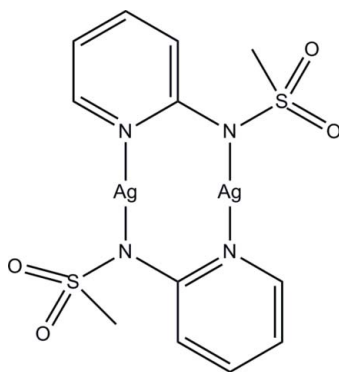
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.036; wR factor = 0.092; data-to-parameter ratio = 32.4.

In the title compound, $[\text{Ag}_2(\text{C}_6\text{H}_7\text{N}_2\text{O}_2\text{S})_2]$, the Ag^{I} atom is coordinated by two N atoms from two *N*-(pyridin-2-yl)methanesulfonamidate anions in a slightly bent linear geometry [$\text{N}-\text{Ag}-\text{N} = 166.03(7)^\circ$]. The Ag^{I} atoms are bridged by the *N*-(pyridin-2-yl)methanesulfonamidate anions, forming a centrosymmetric dinuclear molecule, in which the $\text{Ag}\cdots\text{Ag}$ distance is 2.7072 (4) Å.

Related literature

For related di(pyridyl/pyrimidyl)amide structures, see: Hu *et al.* (2004); Hsu *et al.* (2008); Yeh *et al.* (2008); Tsai *et al.* (2010). For related methyl-4-(pyridin-pyrimidin-2-ylcarbamoyle)benzoate structures, see: Wu *et al.* (2011); Hsiao *et al.* (2012). For related phosphinic amide structures, see: Yeh & Chen (2011); Yeh *et al.* (2012).



Experimental

Crystal data

 $[\text{Ag}_2(\text{C}_6\text{H}_7\text{N}_2\text{O}_2\text{S})_2]$ $M_r = 558.13$

Monoclinic, $P2_1/c$
 $a = 6.4406(2)$ Å
 $b = 15.4580(5)$ Å
 $c = 8.0789(2)$ Å
 $\beta = 97.143(2)^\circ$
 $V = 798.08(4)$ Å³

$Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 2.74$ mm⁻¹
 $T = 296$ K
 $0.20 \times 0.10 \times 0.10$ mm

Data collection

Bruker APEXII CCD area-detector diffractometer
 Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
 $T_{\text{min}} = 0.636$, $T_{\text{max}} = 0.747$

12917 measured reflections
 3569 independent reflections
 2732 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.048$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.092$
 $S = 1.05$
 3569 reflections

110 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 1.32$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.22$ e Å⁻³

Table 1

Selected bond lengths (Å).

Ag—N1	2.1373 (19)	Ag—N2 ⁱ	2.1654 (19)
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Symmetry code: (i) $-x, -y + 1, -z + 1$.

Data collection: *APEX2* (Bruker, 2010); cell refinement: *S SAINT* (Bruker, 2010); data reduction: *S SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); 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: XU5753).

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supporting information

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Bis[μ -*N*-(pyridin-2-yl)methanesulfonamido- κ^2 *N:N'*]silver(I)**Hui-Ling Hu and Chun-Wei Yeh****S0.1. Synthesis and crystallization**

An aqueous solution (5.0 ml) of AgNO₃ (1.0 mmol) was layered carefully over a methanolic solution (5.0 ml) of *N*-(pyridin-2-yl)methanesulfonamide (1.0 mmol) in a tube and kept it in the dark. Colourless crystals were obtained after several weeks. These were washed with methanol and collected in 78.6% yield.

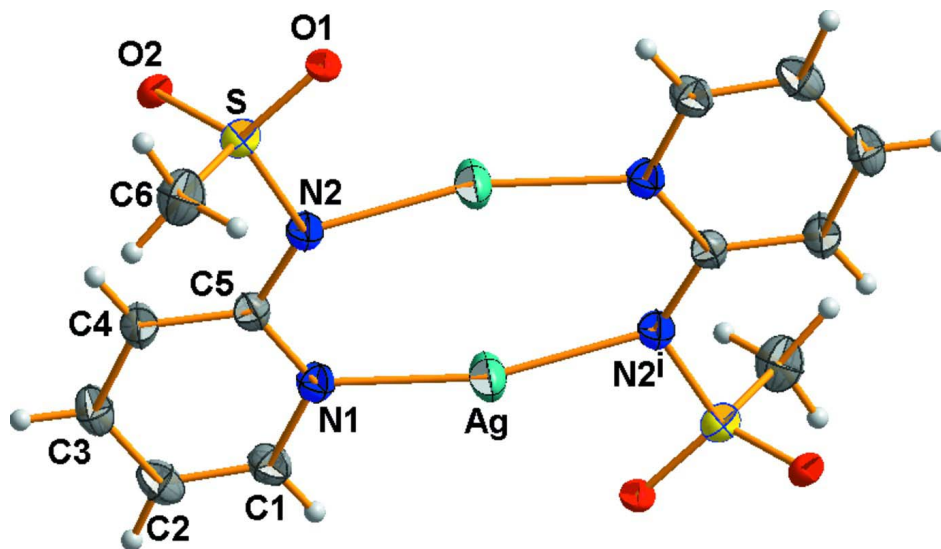
S0.2. Refinement

H atoms were placed in idealized positions and constrained to ride on their parent atoms with C—H = 0.93 or 0.96 Å, U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and 1.2U_{eq}(C) for the others.

S1. Results and discussion

A series of complexes with the symmetric di(pyridyl/pyrimidyl)amide ligands (Hu *et al.*, 2004; Hsu *et al.*, 2008; Yeh *et al.*, 2008; Tsai *et al.*, 2010) and the asymmetric methyl-4-(pyridin-/pyrimidin-2-ylcarbamoyl)benzoate (Wu *et al.*, 2011; Hsiao *et al.*, 2012) or phosphinic amide (Yeh & Chen, 2011; Yeh *et al.*, 2012) ligands that exhibit interesting structural types have been synthesized and structurally characterized. These pyridyl/pyrimidyl amide ligands coordinate to the metal centers through their pyridyl/pyrimidyl nitrogen atoms and/or amide oxygen atoms and interact with each other through hydrogen bonds involving the amide groups. These interactions are important for molecular recognition and constructing supramolecular arrays. .

In the title compound, [Ag(C₆H₇N₂SO₂)₂], the Ag⁺ cations are coordinated with one pyridyl N and one amido N atoms from two *N*-(pyridin-2-yl)methanesulfonamido (*L*-) anions forming a slightly bent geometry (Fig. 1). The Ag...Ag distance separated by the bridging *L*- group is 2.7072 (4) Å.

**Figure 1**

Crystal structure of the title compound with labeling and displacement ellipsoids drawn at 30% probability level.

[Symmetry codes: (i) $-x, -y + 1, -z + 1$.]

Bis[μ -N-(pyridin-2-yl)methanesulfonamido- κ^2 N:N']silver(I)

Crystal data

[Ag₂(C₆H₇N₂O₂S)₂]

$M_r = 558.13$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2ybc$

$a = 6.4406$ (2) Å

$b = 15.4580$ (5) Å

$c = 8.0789$ (2) Å

$\beta = 97.143$ (2)°

$V = 798.08$ (4) Å³

$Z = 2$

$F(000) = 544$

$D_x = 2.323$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 6474 reflections

$\theta = 2.6$ – 35.3 °

$\mu = 2.74$ mm⁻¹

$T = 296$ K

Column, colourless

$0.20 \times 0.10 \times 0.10$ mm

Data collection

Bruker APEXII CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

phi and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2000)

$T_{\min} = 0.636$, $T_{\max} = 0.747$

12917 measured reflections

3569 independent reflections

2732 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.048$

$\theta_{\max} = 35.4$ °, $\theta_{\min} = 2.6$ °

$h = -10 \rightarrow 8$

$k = -25 \rightarrow 22$

$l = -13 \rightarrow 11$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.036$

$wR(F^2) = 0.092$

$S = 1.05$

3569 reflections

110 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0368P)^2 + 0.3136P]$
 where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 1.32 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -1.22 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ag	0.13566 (3)	0.475803 (15)	0.63351 (2)	0.03999 (8)
S	0.07511 (10)	0.64837 (4)	0.14689 (7)	0.02803 (12)
C1	0.5244 (4)	0.58574 (16)	0.6741 (3)	0.0306 (4)
H1A	0.5410	0.5553	0.7742	0.037*
C2	0.6811 (4)	0.64120 (18)	0.6425 (3)	0.0354 (5)
H2A	0.8011	0.6483	0.7181	0.043*
C3	0.6530 (4)	0.68622 (16)	0.4931 (3)	0.0357 (5)
H3A	0.7560	0.7241	0.4664	0.043*
C4	0.4738 (4)	0.67511 (16)	0.3846 (3)	0.0318 (5)
H4A	0.4547	0.7060	0.2851	0.038*
C5	0.3186 (3)	0.61698 (14)	0.4237 (3)	0.0245 (4)
C6	0.2438 (5)	0.6112 (2)	0.0057 (3)	0.0422 (6)
H6A	0.2090	0.6393	-0.1001	0.063*
H6B	0.2281	0.5498	-0.0083	0.063*
H6C	0.3860	0.6243	0.0487	0.063*
N1	0.3482 (3)	0.57273 (12)	0.5690 (2)	0.0255 (3)
N2	0.1362 (3)	0.59867 (13)	0.3207 (2)	0.0274 (4)
O1	-0.1324 (3)	0.61682 (13)	0.0849 (2)	0.0406 (4)
O2	0.1003 (3)	0.74049 (12)	0.1604 (3)	0.0402 (4)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag	0.03197 (12)	0.05057 (14)	0.03650 (11)	-0.01463 (8)	0.00059 (8)	0.01295 (8)
S	0.0278 (3)	0.0277 (3)	0.0283 (3)	0.0004 (2)	0.00232 (19)	0.00570 (19)
C1	0.0274 (11)	0.0352 (12)	0.0286 (10)	-0.0003 (9)	0.0011 (8)	-0.0004 (8)
C2	0.0271 (12)	0.0397 (13)	0.0381 (13)	-0.0043 (10)	-0.0016 (9)	-0.0069 (10)
C3	0.0319 (12)	0.0328 (11)	0.0426 (13)	-0.0105 (10)	0.0054 (10)	-0.0031 (10)
C4	0.0300 (12)	0.0317 (11)	0.0337 (11)	-0.0076 (9)	0.0040 (9)	0.0033 (9)
C5	0.0227 (10)	0.0246 (9)	0.0267 (9)	-0.0013 (7)	0.0047 (7)	-0.0011 (7)
C6	0.0492 (17)	0.0462 (15)	0.0330 (12)	-0.0013 (12)	0.0125 (11)	-0.0002 (10)
N1	0.0251 (9)	0.0272 (9)	0.0245 (8)	-0.0005 (7)	0.0041 (6)	0.0009 (6)

N2	0.0242 (9)	0.0306 (9)	0.0272 (8)	-0.0035 (7)	0.0017 (7)	0.0060 (7)
O1	0.0325 (10)	0.0472 (11)	0.0388 (10)	-0.0050 (8)	-0.0082 (8)	0.0109 (8)
O2	0.0416 (11)	0.0275 (8)	0.0506 (11)	0.0033 (7)	0.0028 (9)	0.0078 (7)

Geometric parameters (Å, °)

Ag—N1	2.1373 (19)	C2—H2A	0.9300
Ag—N2 ⁱ	2.1654 (19)	C3—C4	1.370 (4)
Ag—Ag ⁱ	2.7072 (4)	C3—H3A	0.9300
S—O2	1.4359 (19)	C4—C5	1.409 (3)
S—O1	1.452 (2)	C4—H4A	0.9300
S—N2	1.6061 (19)	C5—N1	1.351 (3)
S—C6	1.766 (3)	C5—N2	1.382 (3)
C1—N1	1.345 (3)	C6—H6A	0.9600
C1—C2	1.372 (4)	C6—H6B	0.9600
C1—H1A	0.9300	C6—H6C	0.9600
C2—C3	1.385 (4)	N2—Ag ⁱ	2.1654 (19)
N1—Ag—N2 ⁱ	166.03 (7)	C3—C4—C5	120.1 (2)
N1—Ag—Ag ⁱ	88.95 (5)	C3—C4—H4A	120.0
N2 ⁱ —Ag—Ag ⁱ	80.07 (5)	C5—C4—H4A	120.0
O2—S—O1	116.73 (12)	N1—C5—N2	115.93 (19)
O2—S—N2	113.24 (11)	N1—C5—C4	119.3 (2)
O1—S—N2	104.81 (11)	N2—C5—C4	124.7 (2)
O2—S—C6	107.40 (13)	S—C6—H6A	109.5
O1—S—C6	106.38 (14)	S—C6—H6B	109.5
N2—S—C6	107.79 (13)	H6A—C6—H6B	109.5
N1—C1—C2	123.9 (2)	S—C6—H6C	109.5
N1—C1—H1A	118.0	H6A—C6—H6C	109.5
C2—C1—H1A	118.0	H6B—C6—H6C	109.5
C1—C2—C3	117.2 (2)	C1—N1—C5	119.3 (2)
C1—C2—H2A	121.4	C1—N1—Ag	117.82 (15)
C3—C2—H2A	121.4	C5—N1—Ag	122.74 (15)
C4—C3—C2	120.2 (2)	C5—N2—S	121.75 (15)
C4—C3—H3A	119.9	C5—N2—Ag ⁱ	130.60 (14)
C2—C3—H3A	119.9	S—N2—Ag ⁱ	106.75 (10)

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