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ISSN 2414-3146

catena-Poly[silver(I)-μ-[1-(pyridin-2-ylmethyl-κN)-3-(3-sulfonatopropyl)imidazolin-2-ylidene]-κC^2]

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Received 18 January 2016
Accepted 9 February 2016

Edited by W. T. A. Harrison, University of Aberdeen, Scotland

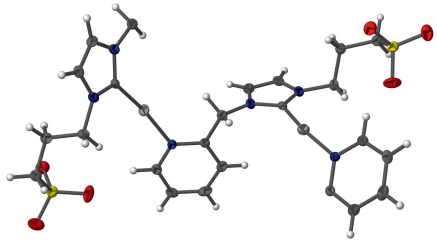
Keywords: crystal structure; one-dimensional helical coordination polymer; silver(I); imidazolinylidene.

CCDC reference: 1452331

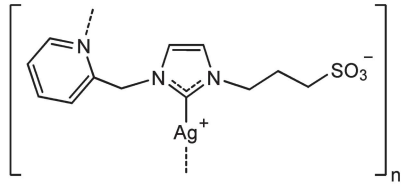
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $[Ag(C_{12}H_{14}N_3O_3S)]_n$, was obtained by deprotonation and metalation of 1-(pyridin-2-ylmethyl)-3-(3-sulfopropyl)imidazolium, inner salt, using silver(I) oxide in methanol. The title compound is a one-dimensional helical coordination polymer. Several C—H···O hydrogen bonds and a short Ag—O contact are observed. The C—Ag—N angle is 168.3 (1)° and the N—C—N 'carbene angle' is 103.8 (3)°.

3D view



Chemical scheme



Structure description

N-Heterocyclic carbene (NHC)–silver complexes are valuable transmetalation reagents or, in other words, carbene transfer agents for the conversion to other metal NHC systems (Lin *et al.*, 2009). Recently, the structural diversity of Ag^I–NHC complexes with pyridyl-substituted imidazolium ligands was discussed in terms of different metal-to-ligand ratios. Increasing degrees of coordination completeness culminated in a polymeric structure (Cui *et al.*, 2012).

In the crystal structure of the title compound, the central C1—Ag—N3^i [symmetry code: (i) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$] bonds deviate considerably from linearity with an angle of 168.3 (1)°, and the dihedral angle between the heterocyclic rings is 50.2 (2)°. The molecular structure is shown in Fig. 1. The N—C—N 'carbene angle' is 103.8 (3)°, in accordance with the mean value of 104.0° in imidazol-2-ylidene–Ag–pyridine complexes from the CSD (119 values from 20 entries). The carbene–metal C1—Ag and nitrogen–metal N3—Ag bonds are 2.065 (4) and 2.144 (3) Å long, respectively, among the shortest in those complexes. The molecules of the title compound form a one-dimensional, helical coordination polymer (Fig. 2). Several C—H···O hydrogen bonds (Table 1) and a short Ag—O contact [2.913 (3) Å] are observed (Fig. 3).

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

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10···O3^{iii}	0.95	2.40	3.349 (4)	173
C6—H6A···O2^{iv}	0.99	2.51	3.458 (5)	160
C7—H7B···O3^{v}	0.99	2.38	3.367 (5)	175
C2—H2···O2^{vi}	0.95	2.53	3.179 (5)	126
C12—H12···O1^{vii}	0.95	2.47	3.143 (4)	128
C7—H7A···O3^{viii}	0.99	2.41	3.257 (4)	143

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

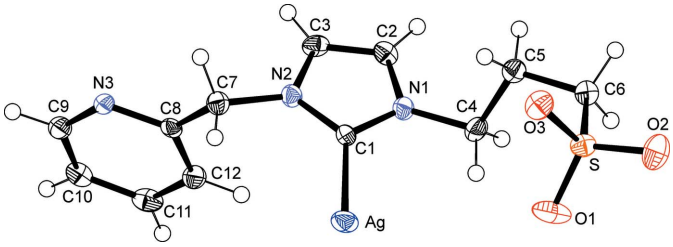


Figure 1
The asymmetric unit of the title compound, showing the atom labels and 50% probability displacement ellipsoids for non-H atoms.

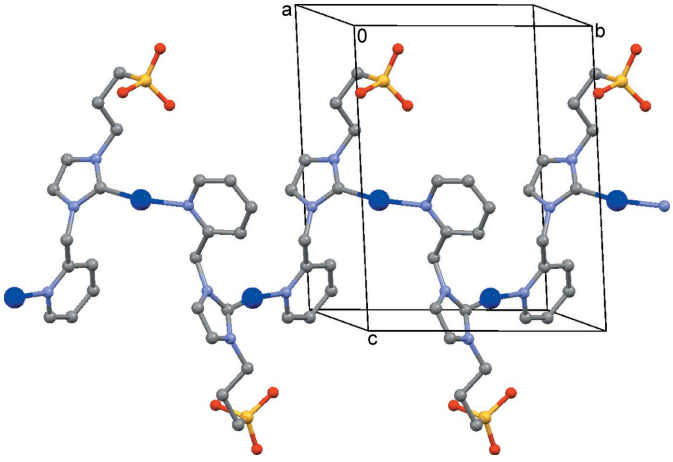


Figure 2
The molecules of the title compound forming a one-dimensional, helical coordination polymer. H atoms have been omitted for clarity.

For related structures, see: Catalano & Moore (2005), Garrison *et al.* (2005), Liu *et al.* (2007), Ye *et al.* (2008), Catalano *et al.* (2011) and Cui *et al.* (2012). These authors describe other structural motifs with polydentate ligands forming NHC–silver complexes.

Synthesis and crystallization

A suspension of the imidazolium salt (0.40 g, 1.4 mmol) (Tomás-Mendivil *et al.*, 2013) and Ag_2O (0.17 g, 0.7 mmol) in MeOH (15 ml) was stirred at room temperature for 18 h. The

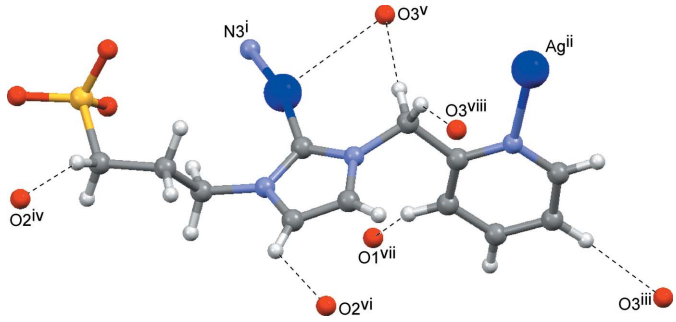


Figure 3
Short contacts in the crystal structure of the title compound. [Symmetry codes: (i) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$. For other symmetry codes, see Table 1].

product was collected by filtration, washed with MeOH and Et_2O and dried to yield colourless crystals (0.44 g, 80%). The PXRD (Cu $K\alpha$ radiation) of the bulk material is identical to the one calculated from the single-crystal diffraction data (Fig. 4), indicating phase purity.

Melting point: 247–252°C. ^{1}H NMR (300 MHz, D_2O): δ 2.24 (*m*, 2H), 2.84 (*m*, 2H), 4.30 (*t*, J = 6.7 Hz, 2H), 5.67 (*s*, 2H), 7.45 (*s*, 1H), 7.51–7.56 (*m*, 2H), 7.87 (*d*, J = 7.6 Hz, 1H), 8.12 (*t*, J = 7.7 Hz, 1H), 8.23 (*m*, 1H) p.p.m. ^{13}C NMR (75 MHz, D_2O): δ 26.8, 47.8, 50.4, 57.8, 123.8, 125.0, 125.8, 126.5, 141.2, 152.3, 154.1, 174.1 p.p.m. IR (neat, ATR): ν 1597 (*w*), 1439 (*w*), 1418

Table 2
Experimental details.

Crystal data	
Chemical formula	[Ag($C_{12}H_{14}N_3O_3S$)]
M_r	388.19
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	173
a, b, c (Å)	11.1568 (6), 9.7852 (4), 12.5715 (6)
β (°)	107.055 (10)
V (Å^3)	1312.09 (12)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.71
Crystal size (mm)	0.15 × 0.04 × 0.03
Data collection	
Diffractometer	Agilent Xcalibur Ruby Gemini ultra
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2014)
T_{min}, T_{max}	0.936, 1
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8214, 2398, 1921
R_{int}	0.045
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.602
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.032, 0.066, 1.02
No. of reflections	2398
No. of parameters	181
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.45, −0.38

Computer programs: *CrysAlis PRO* (Agilent, 2014), *SIR2002* (Burla *et al.*, 2003), *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2006).

(*w*), 1205 (*s*), 1157 (*s*), 1135 (*s*), 1035 (*m*), 750 (*m*), 716 (*s*), 577 (*m*), 518 (*s*) cm^{-1}.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

We are grateful to Christoph Langes for the PXRD measurement.

References

Agilent (2014). *CrysAlis PRO*. Agilent Technologies, Santa Clara, California, USA.
Burla, M. C., Camalli, M., Carrozzini, B., Cascarano, G. L., Giacovazzo, C., Polidori, G. & Spagna, R. (2003). *J. Appl. Cryst.* **36**, 1103.
Catalano, V. J. & Moore, A. L. (2005). *Inorg. Chem.* **44**, 6558–6566.
Catalano, V. J., Munro, L. B., Strasser, C. E. & Samin, A. F. (2011). *Inorg. Chem.* **50**, 8465–8476.
Cui, F., Yang, P., Huang, X., Yang, X.-J. & Wu, B. (2012). *Organometallics*, **31**, 3512–3518.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Garrison, J. C., Tessier, C. A. & Youngs, W. J. (2005). *J. Organomet. Chem.* **690**, 6008–6020.
Lin, J. C. Y., Huang, R. T. W., Lee, C. S., Bhattacharyya, A., Hwang, W. S. & Lin, I. J. B. (2009). *Chem. Rev.* **109**, 3561–3598.

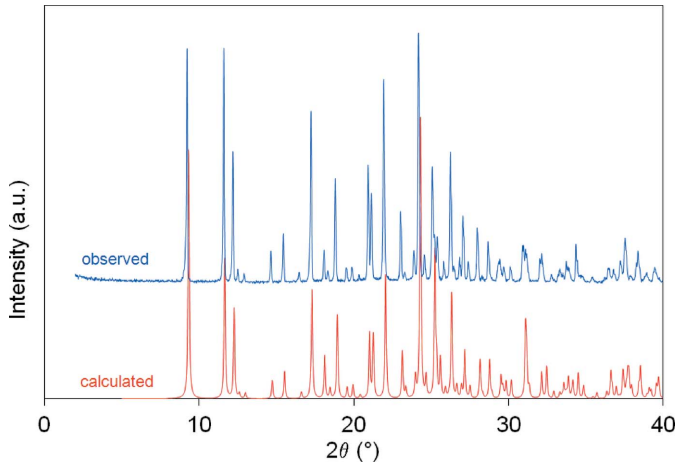


Figure 4
The observed and calculated powder X-ray diffraction data.

Liu, B., Chen, W. & Jin, S. (2007). *Organometallics*, **26**, 3660–3667.
Macrae, C. F., Edgington, P. R., McCabe, P., Pidcock, E., Shields, G. P., Taylor, R., Towler, M. & van de Streek, J. (2006). *J. Appl. Cryst.* **39**, 453–457.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Tomás-Mendivil, E., Toullec, P. Y., Borge, J., Conejero, S., Michelet, V. & Cadierno, V. (2013). *ACS Catal.* **3**, 3086–3098.
Ye, J., Chen, W. & Wang, D. (2008). *Dalton Trans.* pp. 4015–4022.

full crystallographic data

IUCrData (2016). **1**, x160245 [https://doi.org/10.1107/S2414314616002455]

catena-Poly[silver(I)-μ-[1-(pyridin-2-ylmethyl-κN)-3-(3-sulfonatopropyl)-imidazolin-2-ylidene]-κC^2]

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***catena*-Poly[silver(I)-μ-[1-(pyridin-2-ylmethyl-κN)-3-(3-sulfonatopropyl)imidazolin-2-ylidene]-κC^2]**

Crystal data

$[Ag(C_{12}H_{14}N_3O_3S)]$
M_r = 388.19
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 11.1568 (6) Å
b = 9.7852 (4) Å
c = 12.5715 (6) Å
β = 107.055 (10)°
V = 1312.09 (12) Å^3
Z = 4
$F(000)$ = 776
D_x = 1.965 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2698 reflections
θ = 3.6–27.2°
μ = 1.71 mm^{-1}
T = 173 K
Fragment, colourless
0.15 × 0.04 × 0.03 mm

Data collection

Agilent Xcalibur Ruby Gemini ultra diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 10.3575 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2014)
T_{min} = 0.936, T_{max} = 1
8214 measured reflections
2398 independent reflections
1921 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 25.4°, θ_{min} = 2.8°
h = −13→13
k = −11→10
l = −11→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.066
S = 1.02
2398 reflections
181 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
$w = 1/[\sigma^2(F_o^2) + (0.0243P)^2 + 0.580P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Special details

Experimental. Absorption correction: CrysAlisPro, Agilent Technologies, Version 1.171.37.31 (release 14-01-2014 CrysAlis171 .NET) (compiled Jan 14 2014,18:38:05) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ag	0.14608 (3)	0.10604 (3)	0.58234 (2)	0.02486 (11)
S	−0.03575 (9)	0.10338 (8)	0.17887 (8)	0.0211 (2)
N3	0.4721 (3)	−0.2244 (3)	0.9083 (2)	0.0166 (7)
C5	0.1801 (4)	−0.0473 (3)	0.2667 (3)	0.0206 (8)
H5A	0.1213	−0.1022	0.2948	0.025*
H5B	0.2375	−0.1113	0.245	0.025*
N2	0.3417 (3)	−0.1303 (3)	0.6187 (2)	0.0180 (7)
O1	0.0012 (3)	0.2093 (3)	0.2626 (2)	0.0376 (8)
O2	−0.1035 (3)	0.1553 (3)	0.0696 (2)	0.0340 (7)
C11	0.6205 (4)	0.0030 (4)	0.9122 (3)	0.0251 (9)
H11	0.6711	0.0815	0.9136	0.03*
C8	0.4460 (3)	−0.1385 (3)	0.8205 (3)	0.0162 (8)
N1	0.3119 (3)	−0.0352 (3)	0.4606 (2)	0.0189 (7)
C1	0.2724 (4)	−0.0316 (3)	0.5520 (3)	0.0181 (8)
O3	−0.0995 (3)	−0.0096 (2)	0.2142 (2)	0.0279 (6)
C3	0.4222 (3)	−0.1927 (3)	0.5684 (3)	0.0210 (9)
H3	0.4797	−0.2642	0.5987	0.025*
C2	0.4038 (4)	−0.1338 (3)	0.4695 (3)	0.0200 (8)
H2	0.4455	−0.1549	0.4156	0.024*
C10	0.6490 (4)	−0.0863 (3)	1.0009 (3)	0.0217 (8)
H10	0.7202	−0.0721	1.0636	0.026*
C6	0.1058 (4)	0.0317 (3)	0.1644 (3)	0.0210 (8)
H6A	0.085	−0.0302	0.0993	0.025*
H6B	0.1589	0.1063	0.1498	0.025*
C7	0.3302 (4)	−0.1690 (3)	0.7271 (3)	0.0195 (8)
H7A	0.3121	−0.2681	0.7269	0.023*
H7B	0.2584	−0.1195	0.7402	0.023*
C9	0.5710 (4)	−0.1964 (3)	0.9958 (3)	0.0219 (9)
H9	0.5883	−0.256	1.0581	0.026*
C12	0.5181 (4)	−0.0224 (3)	0.8210 (3)	0.0217 (9)
H12	0.4973	0.0387	0.7595	0.026*
C4	0.2562 (4)	0.0444 (3)	0.3597 (3)	0.0237 (9)
H4A	0.3235	0.0897	0.3359	0.028*
H4B	0.2013	0.1162	0.3755	0.028*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag	0.0250 (2)	0.02315 (17)	0.02429 (18)	0.00894 (12)	0.00389 (13)	−0.00441 (11)
S	0.0181 (6)	0.0196 (5)	0.0245 (5)	−0.0014 (4)	0.0046 (4)	−0.0012 (4)
N3	0.0172 (18)	0.0154 (15)	0.0164 (16)	0.0015 (12)	0.0039 (14)	0.0006 (11)
C5	0.019 (2)	0.0209 (18)	0.022 (2)	0.0016 (15)	0.0071 (17)	0.0008 (14)
N2	0.0176 (18)	0.0200 (15)	0.0159 (16)	0.0023 (12)	0.0043 (14)	0.0007 (11)
O1	0.0311 (19)	0.0303 (15)	0.0457 (18)	0.0044 (13)	0.0028 (15)	−0.0195 (12)
O2	0.0238 (18)	0.0409 (16)	0.0336 (17)	0.0025 (13)	0.0028 (14)	0.0114 (12)
C11	0.023 (2)	0.0224 (19)	0.034 (2)	−0.0083 (16)	0.015 (2)	−0.0082 (16)
C8	0.017 (2)	0.0171 (17)	0.0159 (19)	0.0039 (14)	0.0067 (16)	−0.0023 (13)
N1	0.0181 (19)	0.0205 (16)	0.0162 (17)	0.0020 (12)	0.0022 (14)	0.0008 (11)
C1	0.022 (2)	0.0170 (18)	0.0130 (19)	−0.0001 (15)	0.0020 (16)	−0.0014 (13)
O3	0.0248 (17)	0.0280 (14)	0.0334 (16)	−0.0037 (12)	0.0126 (13)	0.0033 (11)
C3	0.015 (2)	0.0190 (18)	0.026 (2)	0.0052 (15)	0.0011 (17)	−0.0022 (15)
C2	0.016 (2)	0.0243 (19)	0.019 (2)	0.0009 (15)	0.0036 (17)	−0.0034 (14)
C10	0.014 (2)	0.027 (2)	0.022 (2)	0.0007 (16)	0.0033 (17)	−0.0062 (15)
C6	0.020 (2)	0.0224 (19)	0.021 (2)	−0.0006 (15)	0.0058 (17)	0.0002 (15)
C7	0.019 (2)	0.0205 (18)	0.019 (2)	−0.0006 (15)	0.0052 (17)	0.0000 (14)
C9	0.024 (2)	0.0205 (19)	0.019 (2)	0.0052 (16)	0.0027 (18)	−0.0005 (14)
C12	0.026 (2)	0.0191 (19)	0.023 (2)	−0.0027 (16)	0.0127 (18)	0.0008 (14)
C4	0.027 (3)	0.0194 (18)	0.021 (2)	0.0036 (16)	0.0016 (18)	0.0039 (14)

Geometric parameters (Å, º)

Ag—C1	2.065 (4)	C8—C12	1.391 (5)
Ag—N3^{i}	2.144 (3)	C8—C7	1.499 (5)
S—O1	1.448 (3)	N1—C1	1.345 (5)
S—O2	1.452 (3)	N1—C2	1.389 (5)
S—O3	1.453 (3)	N1—C4	1.463 (4)
S—C6	1.785 (4)	C3—C2	1.331 (5)
N3—C9	1.338 (5)	C3—H3	0.95
N3—C8	1.350 (4)	C2—H2	0.95
N3—Ag^{ii}	2.144 (3)	C10—C9	1.375 (5)
C5—C4	1.520 (5)	C10—H10	0.95
C5—C6	1.521 (5)	C6—H6A	0.99
C5—H5A	0.99	C6—H6B	0.99
C5—H5B	0.99	C7—H7A	0.99
N2—C1	1.361 (4)	C7—H7B	0.99
N2—C3	1.383 (5)	C9—H9	0.95
N2—C7	1.456 (4)	C12—H12	0.95
C11—C10	1.379 (5)	C4—H4A	0.99
C11—C12	1.383 (5)	C4—H4B	0.99
C11—H11	0.95		
C1—Ag—N3^{i}	168.31 (12)	C2—C3—H3	126.5
O1—S—O2	113.30 (16)	N2—C3—H3	126.5

O1—S—O3	112.50 (17)	C3—C2—N1	106.4 (3)
O2—S—O3	112.94 (17)	C3—C2—H2	126.8
O1—S—C6	106.45 (17)	N1—C2—H2	126.8
O2—S—C6	105.77 (17)	C9—C10—C11	117.8 (3)
O3—S—C6	105.04 (16)	C9—C10—H10	121.1
C9—N3—C8	118.2 (3)	C11—C10—H10	121.1
C9—N3—Ag^{ii}	119.1 (2)	C5—C6—S	113.1 (3)
C8—N3—Ag^{ii}	122.5 (2)	C5—C6—H6A	109
C4—C5—C6	113.1 (3)	S—C6—H6A	109
C4—C5—H5A	108.9	C5—C6—H6B	109
C6—C5—H5A	108.9	S—C6—H6B	109
C4—C5—H5B	108.9	H6A—C6—H6B	107.8
C6—C5—H5B	108.9	N2—C7—C8	112.8 (3)
H5A—C5—H5B	107.8	N2—C7—H7A	109
C1—N2—C3	111.0 (3)	C8—C7—H7A	109
C1—N2—C7	124.8 (3)	N2—C7—H7B	109
C3—N2—C7	124.1 (3)	C8—C7—H7B	109
C10—C11—C12	119.7 (3)	H7A—C7—H7B	107.8
C10—C11—H11	120.1	N3—C9—C10	123.9 (3)
C12—C11—H11	120.1	N3—C9—H9	118.1
N3—C8—C12	121.3 (3)	C10—C9—H9	118.1
N3—C8—C7	116.5 (3)	C11—C12—C8	119.1 (3)
C12—C8—C7	122.1 (3)	C11—C12—H12	120.5
C1—N1—C2	111.7 (3)	C8—C12—H12	120.5
C1—N1—C4	124.4 (3)	N1—C4—C5	110.6 (3)
C2—N1—C4	123.7 (3)	N1—C4—H4A	109.5
N1—C1—N2	103.8 (3)	C5—C4—H4A	109.5
N1—C1—Ag	125.9 (2)	N1—C4—H4B	109.5
N2—C1—Ag	130.1 (3)	C5—C4—H4B	109.5
C2—C3—N2	107.1 (3)	H4A—C4—H4B	108.1

C9—N3—C8—C12	−1.1 (5)	C12—C11—C10—C9	−1.7 (5)
Ag^{ii}—N3—C8—C12	174.2 (3)	C4—C5—C6—S	−79.6 (4)
C9—N3—C8—C7	−176.5 (3)	O1—S—C6—C5	68.0 (3)
Ag^{ii}—N3—C8—C7	−1.3 (4)	O2—S—C6—C5	−171.2 (2)
C2—N1—C1—N2	0.0 (4)	O3—S—C6—C5	−51.5 (3)
C4—N1—C1—N2	174.1 (3)	C1—N2—C7—C8	−115.2 (4)
C2—N1—C1—Ag	175.6 (2)	C3—N2—C7—C8	67.1 (4)
C4—N1—C1—Ag	−10.3 (5)	N3—C8—C7—N2	−147.7 (3)
C3—N2—C1—N1	0.1 (4)	C12—C8—C7—N2	36.9 (5)
C7—N2—C1—N1	−177.9 (3)	C8—N3—C9—C10	−1.1 (5)
C3—N2—C1—Ag	−175.3 (3)	Ag^{ii}—N3—C9—C10	−176.6 (3)
C7—N2—C1—Ag	6.8 (5)	C11—C10—C9—N3	2.5 (6)
N3^{i}—Ag—C1—N1	−26.1 (8)	C10—C11—C12—C8	−0.4 (5)
N3^{i}—Ag—C1—N2	148.3 (5)	N3—C8—C12—C11	1.8 (5)
C1—N2—C3—C2	−0.1 (4)	C7—C8—C12—C11	177.0 (3)
C7—N2—C3—C2	177.9 (3)	C1—N1—C4—C5	−106.9 (4)
N2—C3—C2—N1	0.1 (4)	C2—N1—C4—C5	66.5 (5)

C1—N1—C2—C3	0.0 (4)	C6—C5—C4—N1	172.4 (3)
C4—N1—C2—C3	−174.2 (3)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10···O3^{iii}	0.95	2.40	3.349 (4)	173
C6—H6*A*···O2^{iv}	0.99	2.51	3.458 (5)	160
C7—H7*B*···O3^{v}	0.99	2.38	3.367 (5)	175
C2—H2···O2^{vi}	0.95	2.53	3.179 (5)	126
C12—H12···O1^{vii}	0.95	2.47	3.143 (4)	128
C7—H7*A*···O3^{viii}	0.99	2.41	3.257 (4)	143

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