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Poly[bis(μ_2-cyanido)-κ^2C:N;κ^2N:C-(μ_2-N,N,N',N'-tetramethylthiourea-κ^2S:S)-disilver(I)]

Muhammad Hanif,[a] Saeed Ahmad,[a]* Muhammad Altaf[b] and Helen Stoeckli-Evans[b]

[a]Department of Chemistry, University of Engineering and Technology, Lahore, Pakistan, and [b]Institute of Microtechnology, University of Neuchâtel, Rue Emile-Argand 11, CH-2000 Neuchâtel, Switzerland
Correspondence e-mail: saeed_a786@hotmail.com

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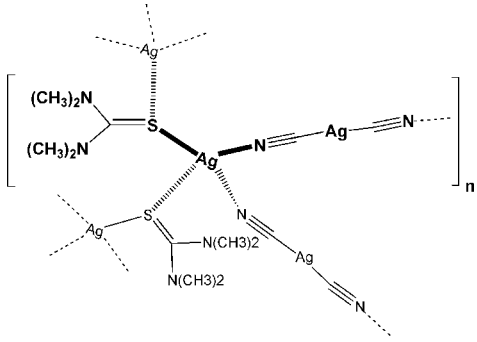
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(N–C) = 0.005 Å; R factor = 0.030; wR factor = 0.070; data-to-parameter ratio = 24.9.

The title compound, $[Ag_2(CN)_2(C_5H_{12}N_2S)]_n$, crystallizes as an infinite three-dimensional framework structure. It exists in an unusual ionic form, the asymmetric unit being composed of a cation $[(\mu$-tetramethylthiourea-S)Ag$]^+$ and an anion $[(Ag(CN)_2]^-$. The thiourea S atom is coordinated asymmetrically to silver ions, linking two almost parallel chains. The same silver atom is linked to a symmetry-related atom by the $[Ag(CN)_2]^-$ anion. In this way, a three-dimensional structure is built up. The shortest Ag···Ag intermolecular contact distance involves the silver atom in the $[Ag(CN)_2]^-$ anion [Ag···Ag 3.6965 (5) Å].

Related literature

For related literature, see: Stocker *et al.* (2000).



Experimental

Crystal data

$[Ag_2(CN)_2(C_5H_{12}N_2S)]$
M_r = 400.01
Orthorhombic, *Pbca*
a = 7.3563 (4) Å
b = 15.6735 (11) Å
c = 20.9978 (16) Å
V = 2421.0 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 3.38 mm^{-1}
T = 173 (2) K
0.20 × 0.20 × 0.10 mm

Data collection

Stoe IPDS-2 diffractometer
Absorption correction: multi-scan (*MULABS* in *PLATON*; Spek, 2003)
T_{min} = 0.402, T_{max} = 0.709
32772 measured reflections
3284 independent reflections
2731 reflections with $I > 2\sigma(I)$
R_{int} = 0.070

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.070
S = 1.07
3284 reflections
132 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.94 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—S1	2.4990 (9)	Ag1—S1^{i}	2.7075 (9)
Ag1—N3	2.288 (3)	Ag2—C6	2.047 (3)
Ag1—N4	2.242 (3)	Ag2—C7^{ii}	2.048 (3)
Ag2···Ag2^{iii}	3.6965 (5)	Ag2···Ag2^{iv}	3.6965 (5)
S1—Ag1—N3	115.62 (9)	S1^{i}—Ag1—N4	102.98 (9)
S1—Ag1—N4	135.76 (9)	C6—Ag2—C7^{ii}	178.41 (13)
S1—Ag1—S1^{i}	94.30 (3)	Ag1—S1—C1	101.51 (12)
N3—Ag1—N4	99.64 (12)	Ag1—S1—Ag1^{v}	147.80 (4)
S1^{i}—Ag1—N3	103.39 (9)	Ag1^{v}—S1—C1	93.32 (12)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5A···N1	0.98	2.52	2.871 (6)	101

Data collection: *X-AREA* (Stoe & Cie, 2005); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); 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: BQ2035).

References

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  doi:10.1107/S1600536807044844

supplementary materials

Acta Cryst. (2007). E**63**, m2594 [**doi:10.1107/S1600536807044844**]

Poly[bis(μ_2-cyanido)-κ^2C:N;κ^2N:C-(μ_2-N,N,N',N'-tetramethylthiourea-κ^2S:S)disilver(I)]

M. Hanif, S. Ahmad, M. Altaf and H. Stoeckli-Evans

Comment

The structure of the asymmetric unit of the title compound is shown in Fig. 1. The reaction of the silver nitrate complex of tetramethylthiourea with KCN lead to the formation of an unusual ionic three dimensional polymer. The asymmetric unit is composed of a cation, $[(\mu\text{-tetramethylthiourea-}S)Ag]^+$, and an anion, $[(Ag(CN)_2]^-$. The S-atom of the cation asymmetrically bridges two silver Ag1 atoms in two almost parallel symmetry related chains; bond distance S1—Ag1 is 2.4990 (9) Å, while distance S1—Ag1^{i} is 2.7075 (9) Å [symmetry operation (i) = $x + 1/2, -y + 1/2, -z$]. The Ag1 atoms in these chains are further linked *via* the N-atoms of the $[(Ag(CN)_2]^-$ anions (Fig. 2), so building up the three dimensional framework.

The Ag1—N(CN) distances are normal [2.288 (3) and 2.242 (3) Å], as are the Ag2—C distances [2.047 (3) and 2.048 (3) Å], indicating no disorder of the C≡N bonds. The reaction of tetramethylthiourea with AgCN lead to the formation of a one-dimensional chiral polymer (Stocker *et al.*, 2000). There the cyanide groups, coordinated to equivalent Ag atoms, have equal distances at both ends (2.155 (4) Å) and are completely disordered.

In the crystal structure the shortest Ag···Ag intermolecular contact distance involves atom Ag2 of the $[Ag(CN)_2]^-$ anion; distance Ag2···Ag2^{iii} is equal to 3.6965 (5) Å [symmetry operation (iii) = $x - 1/2, y, -z - 1/2$].

Experimental

The title compound was prepared by adding 2 mmol of tetramethylthiourea in 15–20 ml of methanol to 1 mmol (0.17 g) of $AgNO_3$, followed by the addition of 1 mmol of KCN dissolved in 15 − 20 ml of distilled water. A clear solution was obtained and was stirred for *ca* 30 min. The solution was filtered and the filtrate allowed to evaporate slowly at room temperature, giving colorless block-like crystals.

Refinement

The H-atoms were included in calculated positions and treated as riding atoms: C—H = 0.98 Å with U_{iso}(H) = 1.5U $_{eq}$ (C).

Figures

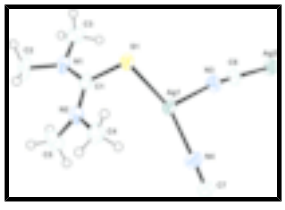

Fig. 1. The asymmetric unit of compound (I), showing the atomic numbering scheme and displacement parameters drawn at the 50% probabilty level.

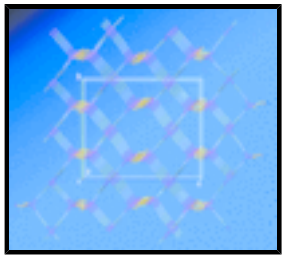

Fig. 2. The crystal packing of compound (I) viewed along the *a* axis. The hydrogen atoms and C and N-atoms of the thiourea moiety have been omitted for clarity.

Poly[di-μ$_2$-cyanido-κ^2*C*:*N*;κ^2*N*:*C*-μ$_2$-*N*,*N*,*N*',*N*'- tetramethylthiourea-κ^2*S*:*S*-disilver(I)]

Crystal data

$[Ag_2(CN)_2(C_5H_{12}N_2S)]$	F_{000} = 1536
M_r = 400.01	D_x = 2.195 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 23959 reflections
a = 7.3563 (4) Å	θ = 1.8–29.6º
b = 15.6735 (11) Å	μ = 3.38 mm^{-1}
c = 20.9978 (16) Å	*T* = 173 (2) K
V = 2421.0 (3) Å^3	Block, colourless
Z = 8	0.20 × 0.20 × 0.10 mm

Data collection

Stoe IPDS-2 diffractometer	3284 independent reflections
Radiation source: fine-focus sealed tube	2731 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.070
T = 173(2) K	θ_{max} = 29.3º
φ and ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (MULscanABS in PLATON; Spek, 2003)	*h* = −10→9
T_{min} = 0.402, T_{max} = 0.709	*k* = −21→21
32772 measured reflections	*l* = −28→28

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.030	$w = 1/[\sigma^2(F_o^2) + (0.0265P)^2 + 3.3418P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.070	$(\Delta/\sigma)_{max} < 0.001$
S = 1.07	$\Delta\rho_{max}$ = 0.46 e Å^{-3}
3284 reflections	$\Delta\rho_{min}$ = −0.94 e Å^{-3}

132 parameters	Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.00073 (8)
Secondary atom site location: difference Fourier map	

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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	0.34332 (3)	0.25371 (2)	−0.08070 (1)	0.0319 (1)
Ag2	0.51946 (4)	−0.00703 (2)	−0.24123 (1)	0.0409 (1)
S1	0.16344 (11)	0.22840 (6)	0.01848 (4)	0.0326 (2)
N1	0.3533 (4)	0.25257 (19)	0.12435 (13)	0.0349 (8)
N2	0.3000 (4)	0.37387 (19)	0.06475 (13)	0.0340 (8)
N3	0.3898 (5)	0.1365 (2)	−0.14355 (15)	0.0412 (10)
N4	0.3563 (5)	0.3562 (2)	−0.15502 (16)	0.0425 (10)
C1	0.2806 (5)	0.2894 (2)	0.07285 (15)	0.0304 (9)
C2	0.3721 (6)	0.2957 (3)	0.18619 (17)	0.0526 (15)
C3	0.3799 (5)	0.1602 (3)	0.1272 (2)	0.0447 (12)
C4	0.1848 (6)	0.4213 (3)	0.02035 (18)	0.0437 (11)
C5	0.4564 (6)	0.4223 (3)	0.0878 (2)	0.0520 (14)
C6	0.4379 (5)	0.0842 (2)	−0.17756 (17)	0.0367 (10)
C7	0.3986 (6)	0.4043 (2)	−0.19317 (17)	0.0378 (10)
H2A	0.30460	0.34960	0.18540	0.0780*
H2B	0.50090	0.30730	0.19450	0.0780*
H2C	0.32340	0.25900	0.21990	0.0780*
H3A	0.26920	0.13310	0.14350	0.0670*
H3B	0.48190	0.14720	0.15560	0.0670*
H3C	0.40620	0.13850	0.08440	0.0670*
H4A	0.06390	0.39510	0.01880	0.0660*
H4B	0.23930	0.42000	−0.02220	0.0660*
H4C	0.17390	0.48060	0.03470	0.0660*
H5A	0.54660	0.38290	0.10560	0.0780*
H5B	0.41690	0.46230	0.12080	0.0780*
H5C	0.51080	0.45400	0.05240	0.0780*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0352 (1)	0.0369 (1)	0.0236 (1)	−0.0003 (1)	0.0017 (1)	−0.0003 (1)
Ag2	0.0590 (2)	0.0348 (1)	0.0290 (1)	0.0060 (1)	−0.0008 (1)	−0.0063 (1)
S1	0.0276 (4)	0.0458 (4)	0.0245 (3)	−0.0063 (3)	0.0019 (3)	−0.0043 (3)
N1	0.0337 (14)	0.0465 (16)	0.0246 (12)	0.0047 (13)	−0.0024 (11)	−0.0015 (12)
N2	0.0328 (15)	0.0401 (15)	0.0292 (13)	0.0021 (12)	−0.0053 (12)	−0.0058 (12)
N3	0.0458 (18)	0.0419 (16)	0.0358 (16)	−0.0038 (13)	0.0028 (14)	−0.0075 (13)
N4	0.0450 (19)	0.0447 (16)	0.0377 (16)	−0.0011 (14)	−0.0037 (14)	0.0085 (14)
C1	0.0268 (14)	0.0400 (17)	0.0243 (14)	0.0031 (13)	0.0021 (12)	−0.0029 (13)
C2	0.056 (3)	0.078 (3)	0.0237 (16)	0.015 (2)	−0.0075 (16)	−0.0088 (18)
C3	0.039 (2)	0.051 (2)	0.044 (2)	0.0043 (16)	−0.0001 (16)	0.0111 (18)
C4	0.048 (2)	0.045 (2)	0.0382 (18)	0.0076 (17)	−0.0065 (17)	0.0007 (16)
C5	0.049 (2)	0.049 (2)	0.058 (3)	−0.0059 (19)	−0.013 (2)	−0.0116 (19)
C6	0.044 (2)	0.0343 (16)	0.0317 (17)	−0.0023 (14)	0.0013 (14)	−0.0039 (14)
C7	0.047 (2)	0.0347 (17)	0.0316 (17)	−0.0025 (15)	−0.0029 (15)	0.0030 (14)

Geometric parameters (Å, °)

Ag1—S1	2.4990 (9)	N4—C7	1.143 (5)
Ag1—N3	2.288 (3)	C2—H2A	0.9800
Ag1—N4	2.242 (3)	C2—H2B	0.9800
Ag1—S1^{i}	2.7075 (9)	C2—H2C	0.9800
Ag2—C6	2.047 (3)	C3—H3A	0.9800
Ag2—C7^{ii}	2.048 (3)	C3—H3B	0.9800
S1—C1	1.721 (3)	C3—H3C	0.9800
N1—C1	1.337 (4)	C4—H4A	0.9800
N1—C2	1.470 (5)	C4—H4B	0.9800
N1—C3	1.462 (6)	C4—H4C	0.9800
N2—C1	1.342 (4)	C5—H5A	0.9800
N2—C4	1.463 (5)	C5—H5B	0.9800
N2—C5	1.461 (5)	C5—H5C	0.9800
N3—C6	1.143 (5)		
Ag1···C4	3.572 (4)	C6···C2^{vi}	3.459 (5)
Ag1···C4^{i}	3.929 (5)	C6···Ag2^{vii}	3.798 (4)
Ag1···C5^{iii}	3.967 (5)	C7···Ag2^{x}	3.523 (4)
Ag1···N1^{iii}	3.721 (3)	C2···H5A	2.5300
Ag1···C1^{iii}	4.198 (4)	C2···H5B	2.9700
Ag1···C2^{iii}	4.186 (4)	C5···H2B	2.8900
Ag1···C3^{iii}	3.794 (4)	C5···H2A	2.6000
Ag1···C3^{i}	4.284 (4)	C6···H2A^{i}	2.8900
Ag2···C6^{iv}	3.798 (4)	C7···H3A^{i}	2.9800
Ag2···C3^{v}	3.471 (4)	C7···H5B^{xii}	2.9200
Ag2···C2^{vi}	3.804 (5)	H2A···N2	2.5600

Ag2···C5^{vi}	3.856 (4)	H2A···C5	2.6000
Ag2···Ag2^{vii}	3.6965 (5)	H2A···H5A	2.5000
Ag2···Ag2^{iv}	3.6965 (5)	H2A···H5B	2.3800
Ag2···N4^{viii}	3.939 (3)	H2A···Ag2^{iii}	3.4400
Ag2···C7^{viii}	3.523 (4)	H2A···C6^{iii}	2.8900
Ag1···H3C^{iii}	3.6300	H2A···Ag2^{xi}	3.3100
Ag1···H4A	3.6700	H2B···C5	2.8900
Ag1···H2B^{iii}	3.6000	H2B···H5A	2.2400
Ag1···H3B^{iii}	3.4600	H2B···Ag1^{i}	3.6000
Ag1···H4A^{i}	3.1200	H2B···Ag2^{xi}	3.4100
Ag1···H5A^{iii}	3.1000	H2C···H3A	2.5700
Ag1···H4B	2.9800	H2C···H3B	2.5000
Ag2···H3A^{ix}	3.7800	H3A···S1	3.1200
Ag2···H2A^{i}	3.4400	H3A···H2C	2.5700
Ag2···H3A^{v}	3.2500	H3A···Ag2^{xiii}	3.7800
Ag2···H3B^{v}	2.8400	H3A···C7^{iii}	2.9800
Ag2···H2A^{vi}	3.3100	H3A···Ag2^{v}	3.2500
Ag2···H2B^{vi}	3.4100	H3B···H2C	2.5000
Ag2···H5A^{vi}	3.7600	H3B···Ag1^{i}	3.4600
Ag2···H5B^{vi}	3.0700	H3B···N4^{i}	2.7500
S1···C1^{iii}	3.419 (4)	H3B···Ag2^{v}	2.8400
S1···C5^{iii}	3.589 (5)	H3C···S1	2.6600
S1···H3A	3.1200	H3C···Ag1^{i}	3.6300
S1···H4B	3.1700	H3C···H4A^{i}	2.5100
S1···H3C	2.6600	H4A···Ag1	3.6700
S1···H4A	2.7100	H4A···S1	2.7100
N1···Ag1^{i}	3.721 (3)	H4A···Ag1^{iii}	3.1200
N3···C1^{i}	3.438 (5)	H4A···H3C^{iii}	2.5100
N4···Ag2^{x}	3.939 (3)	H4B···Ag1	2.9800
N1···H5A	2.5200	H4B···S1	3.1700
N2···H2A	2.5600	H4B···H5C	2.5900
N3···H5A^{iii}	2.6600	H4C···H5B	2.5600
N4···H3B^{iii}	2.7500	H4C···H5C	2.5400
C1···Ag1^{i}	4.198 (4)	H5A···N1	2.5200
C2···C5	2.931 (6)	H5A···C2	2.5300
C2···Ag2^{xi}	3.804 (5)	H5A···H2A	2.5000
C2···C6^{xi}	3.459 (5)	H5A···H2B	2.2400
C2···Ag1^{i}	4.186 (4)	H5A···Ag1^{i}	3.1000
C3···Ag2^{v}	3.471 (4)	H5A···N3^{i}	2.6600
C3···Ag1^{iii}	4.284 (4)	H5A···Ag2^{xi}	3.7600
C3···Ag1^{i}	3.794 (4)	H5B···C2	2.9700
C4···Ag1	3.572 (4)	H5B···H2A	2.3800

C4···Ag1^{iii}	3.929 (5)	H5B···H4C	2.5600
C5···Ag2^{xi}	3.856 (4)	H5B···C7^{xii}	2.9200
C5···S1^{i}	3.589 (5)	H5B···Ag2^{xi}	3.0700
C5···C2	2.931 (6)	H5C···H4B	2.5900
C5···Ag1^{i}	3.967 (5)	H5C···H4C	2.5400
S1—Ag1—N3	115.62 (9)	N1—C2—H2B	109.00
S1—Ag1—N4	135.76 (9)	N1—C2—H2C	109.00
S1—Ag1—S1^{i}	94.30 (3)	H2A—C2—H2B	109.00
N3—Ag1—N4	99.64 (12)	H2A—C2—H2C	109.00
S1^{i}—Ag1—N3	103.39 (9)	H2B—C2—H2C	109.00
S1^{i}—Ag1—N4	102.98 (9)	N1—C3—H3A	109.00
C6—Ag2—C7^{ii}	178.41 (13)	N1—C3—H3B	109.00
Ag1—S1—C1	101.51 (12)	N1—C3—H3C	109.00
Ag1—S1—Ag1^{iii}	147.80 (4)	H3A—C3—H3B	109.00
Ag1^{iii}—S1—C1	93.32 (12)	H3A—C3—H3C	109.00
C1—N1—C2	123.6 (3)	H3B—C3—H3C	110.00
C1—N1—C3	120.9 (3)	N2—C4—H4A	110.00
C2—N1—C3	114.0 (3)	N2—C4—H4B	109.00
C1—N2—C4	121.4 (3)	N2—C4—H4C	109.00
C1—N2—C5	123.7 (3)	H4A—C4—H4B	109.00
C4—N2—C5	113.8 (3)	H4A—C4—H4C	109.00
Ag1—N3—C6	169.2 (3)	H4B—C4—H4C	109.00
Ag1—N4—C7	166.4 (3)	N2—C5—H5A	109.00
S1—C1—N1	119.8 (2)	N2—C5—H5B	109.00
S1—C1—N2	121.2 (2)	N2—C5—H5C	110.00
N1—C1—N2	119.1 (3)	H5A—C5—H5B	110.00
Ag2—C6—N3	177.8 (3)	H5A—C5—H5C	109.00
Ag2^{xiv}—C7—N4	177.7 (3)	H5B—C5—H5C	109.00
N1—C2—H2A	109.00		
N3—Ag1—S1—C1	139.11 (15)	Ag1—S1—C1—N1	−120.5 (3)
N3—Ag1—S1—Ag1^{iii}	−105.15 (12)	Ag1—S1—C1—N2	59.8 (3)
N4—Ag1—S1—C1	−81.55 (18)	Ag1^{iii}—S1—C1—N1	88.3 (3)
N4—Ag1—S1—Ag1^{iii}	34.19 (16)	Ag1^{iii}—S1—C1—N2	−91.4 (3)
S1^{i}—Ag1—S1—C1	32.04 (12)	C2—N1—C1—S1	−148.1 (3)
S1^{i}—Ag1—S1—Ag1^{iii}	147.78 (7)	C2—N1—C1—N2	31.6 (5)
S1—Ag1—S1^{i}—Ag1^{i}	18.94 (8)	C3—N1—C1—S1	17.1 (5)
S1—Ag1—S1^{i}—C1^{i}	136.79 (11)	C3—N1—C1—N2	−163.2 (3)
N3—Ag1—S1^{i}—Ag1^{i}	−98.68 (11)	C4—N2—C1—S1	16.8 (5)
N3—Ag1—S1^{i}—C1^{i}	19.17 (14)	C4—N2—C1—N1	−162.9 (3)
N4—Ag1—S1^{i}—Ag1^{i}	157.94 (11)	C5—N2—C1—S1	−149.9 (3)
N4—Ag1—S1^{i}—C1^{i}	−84.21 (14)	C5—N2—C1—N1	30.4 (5)

Symmetry codes: (i) *x*+1/2, −*y*+1/2, −*z*; (ii) −*x*+1, *y*−1/2, −*z*−1/2; (iii) *x*−1/2, −*y*+1/2, −*z*; (iv) *x*+1/2, *y*, −*z*−1/2; (v) −*x*+1, −*y*, −*z*; (vi) *x*, −*y*+1/2, *z*−1/2; (vii) *x*−1/2, *y*, −*z*−1/2; (viii) −*x*+1/2, *y*−1/2, *z*; (ix) −*x*+1/2, −*y*, *z*−1/2; (x) −*x*+1/2, *y*+1/2, *z*; (xi) *x*, −*y*+1/2, *z*+1/2; (xii) −*x*+1, −*y*+1, −*z*; (xiii) −*x*+1/2, −*y*, *z*+1/2; (xiv) −*x*+1, *y*+1/2, −*z*−1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5A···N1	0.98	2.52	2.871 (6)	101

Fig. 1

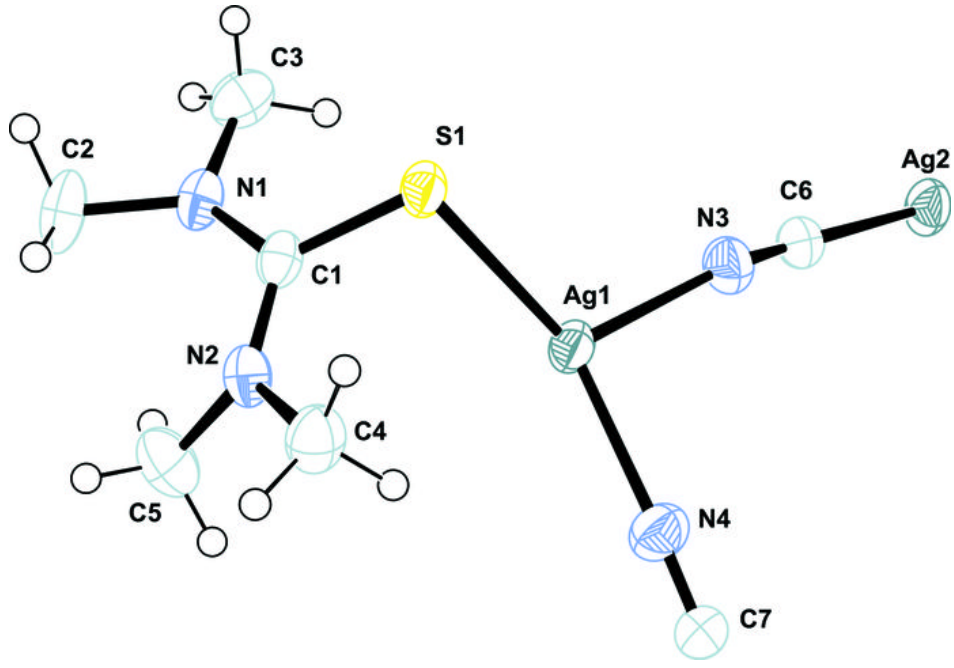

Fig. 2