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Bis[bis(1*H*-imidazole-κN^3)silver(I)] naphthalene-1,5-disulfonate

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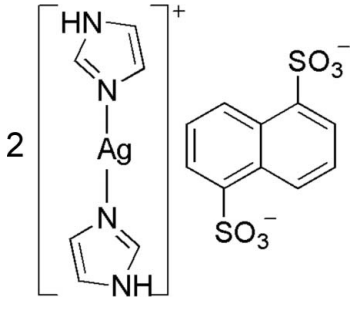
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.026; wR factor = 0.063; data-to-parameter ratio = 16.4.

The title compound, $[Ag(C_3H_4N_2)_2]_2(C_{10}H_6O_6S_2)$, exists in the form of isolated cations and anions with electrostatic interaction between them. The Ag atom is two-coordinated by the N atoms of two crystallographically independent imidazole molecules. The naphthalene-1,5-disulfonate anion is located on a crystallographic center of symmetry. The cations and anions are connected through intermolecular N—H···O hydrogen bonds.

Related literature

For related literature, see: Côté & Shimizu (2003, 2004); Cai (2004); Cai *et al.* (2001); Chen *et al.* (2001, 2002); Dalrymple & Shimizu (2002); Lian *et al.* (2007); Liu *et al.* (2006); Reddy *et al.* (2003); Shimizu *et al.* (1999); Zhou *et al.* (2004).



Experimental

Crystal data

$[Ag(C_3H_4N_2)_2]_2(C_{10}H_6O_6S_2)$
M_r = 774.36
Triclinic, $P\overline{1}$
a = 8.6491 (11) Å
b = 9.0196 (12) Å
c = 10.2620 (13) Å
α = 65.286 (2)°
β = 76.311 (2)°
γ = 66.791 (2)°
V = 665.89 (15) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.68 mm^{-1}
T = 293 (2) K
0.50 × 0.30 × 0.13 mm

Data collection

Bruker Smart 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.487, T_{max} = 0.811
4267 measured reflections
2962 independent reflections
2417 reflections with $I > 2\sigma(I)$
R_{int} = 0.010

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.063
S = 0.93
2962 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.70 e Å^{-3}
$\Delta\rho_{min}$ = −0.67 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4A···O2^{i}	0.86	1.96	2.786 (3)	161
N2—H2A···O3^{ii}	0.86	2.37	2.998 (3)	130
N2—H2A···O3^{iii}	0.86	2.32	3.082 (3)	149

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2068).

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Ping Liu and Dong-Sheng Deng

S1. Comment

In the part of our recent investigations into the development of mixed inorganic–organic hybrid materials, we synthesized the silver sulfonate compound, which can be possess a potential wide chemical opportunity.

Sulfonate compounds have received much attention due to their potential application in chemical absorption and separation (Cai *et al.*, 2004; Zhou *et al.*, 2004; Liu *et al.*, 2006). However, the weak coordination nature of SO_3–group makes its coordination mode very flexible and sensitive to the chemical environment (Côté *et al.*, 2003). Likewise, Ag^+ ion is a notoriously pliant with respect to its coordination sphere. Thus, in silver sulfonates, various coordination modes are observed with coordination number ranging from two to nine (Côté *et al.*, 2004; Dalrymple *et al.*, 2002; Reddy *et al.*, 2003; Shimizu *et al.*, 1999). On the other hand, the coordination behavior of arene–sulfonates with transition metals can be peculiar in the presence of amino ligands (Chen *et al.*, 2001; Cai *et al.*, 2001; Chen *et al.*, 2002).

The structure of the title compound, (**I**), is depicted in Fig. 1. There is one crystallographically independent Ag centre, coordinated by two nitrogen atoms from two different imidazole ligands with Ag—N1 = 2.1088 (19)Å and Ag—N2 = 2.109 (2) Å, respectively. The lesser contact distance Ag···O1 = 2.8185 (19)Å is longer than the reported Ag···O distance (Lian *et al.*, 2007).

Cations and anions are connected through intermolecular N—H···O hydrogen bonds to form a linear tapes (N4—H4A···O2^{ii}): N4···O2^{ii} = 2.786 (3) Å, H4A···O2^{ii} = 1.96Å and angle N4—H4A···O2^{ii} = 160.7°, which run along the *a*–axis. The linear tapes are arranged in parallel fashion and further linked *via* hydrogen bonding between the coordinated imidazole molecules and the sulfonate oxygen atoms, thus leading to neutral extended two–dimensional sheets (N2—H2A···O3^{iii}): N2···O3^{iii} = 2.998 (3) Å, angle N2—H2A···O3^{iii} = 129.8° and (N2—H2A···O3^{iv}): N2···O3^{iv} = 3.082 (3) Å, angle N2—H2A···O3^{iv} = 148.6° as shown on Fig. 2 (symmetry codes: (ii) 1 + *x*, *y*, *z*); (iii) *x* - 2, *y* + 1, *z*; (iv) -*x*, 2 - *y*, 2 - *z*).

S2. Experimental

Disodium 1,5–naphthalene–disulfonate (0.33 g, 1 mmol) and imidazole (0.27 g, 4 mmol) were added to an aqueous solution of $AgNO_3$ (0.32 g, 2 mmol) (10 ml). The result solution was stirred at 343 K for four hours in a water bath. After filtration, a clear solution was set aside to crystallize.

S3. Refinement

All H atoms were positioned geometrically and treated as riding, with C—H = 0.93 Å, N—H = 0.86 Å, respectively, and with U_{iso}(H) = 1.2U_{eq}(C or N)

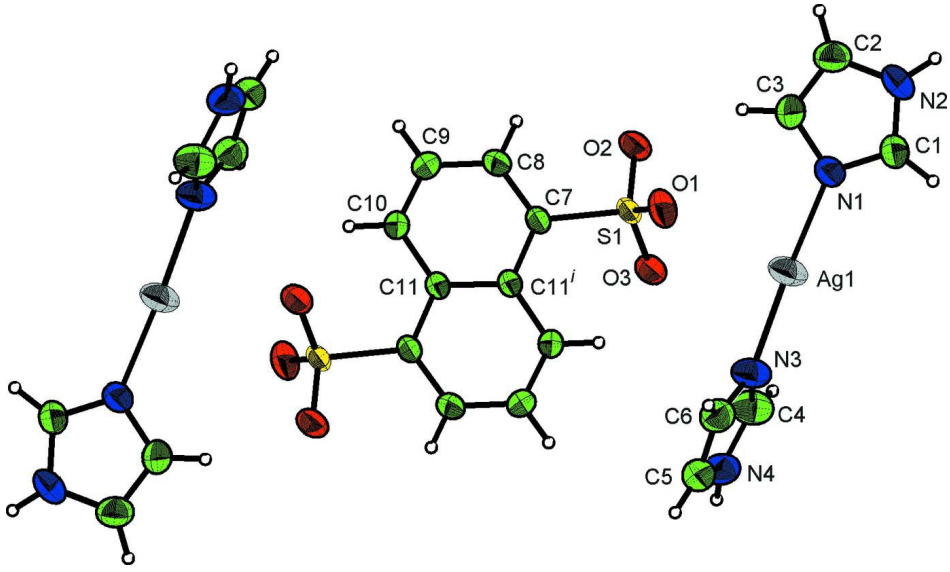

Figure 1

Molecular structure of **I** with the numbering scheme. Displacement ellipsoids are drawn at 30% probability level. H atoms are presented as a small spheres with arbitrary radius. Symmetry code: (i) 1 - *x*, 1 - *y*, 1 - *z*.

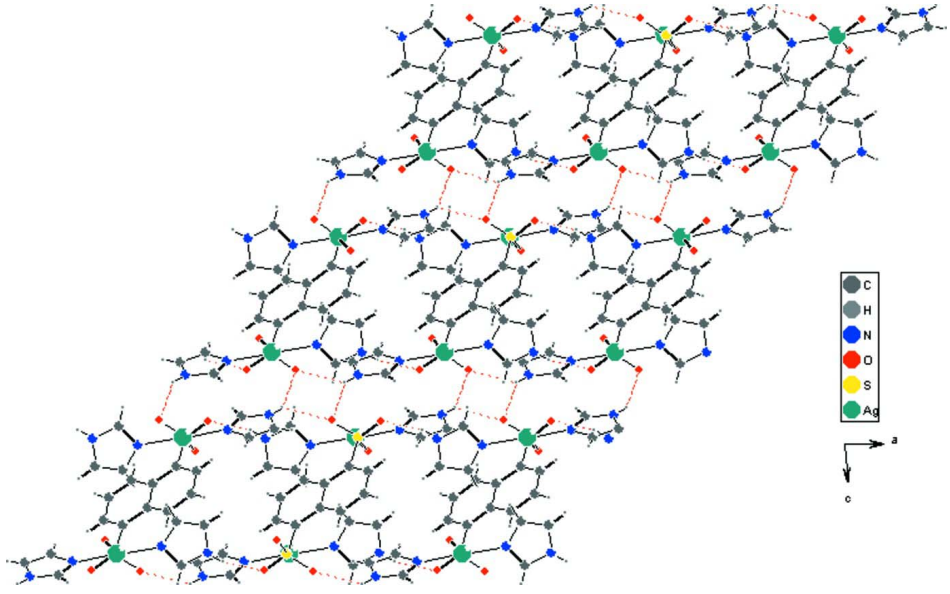

Figure 2

View of the sheet structure of **I** normal to the *ac*–plane. Hydrogen bonds are represented as dashed lines.

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Hall symbol: -P 1
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$b = 9.0196$ (12) Å
$c = 10.2620$ (13) Å
$\alpha = 65.286$ (2)°
$\beta = 76.311$ (2)°
$\gamma = 66.791$ (2)°
$V = 665.89$ (15) Å^3
$Z = 1$

$F(000) = 384$
$D_x = 1.931$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2962 reflections
$\theta = 2.2–27.5°$
$\mu = 1.68$ mm^{-1}
$T = 293$ K
Block, colourless
0.50 × 0.30 × 0.13 mm

Data collection

Bruker Smart 1000 CCD diffractometer
Radiation source: Fine–focus sealed tube
Graphite monochromator
φ– and ω–scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.487$, $T_{max} = 0.811$
4267 measured reflections
2962 independent reflections
2417 reflections with $I > 2\sigma(I)$
$R_{int} = 0.010$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.2°$
$h = -11 \rightarrow 9$
$k = -11 \rightarrow 10$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.063$
$S = 0.93$
2962 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
$w = 1/[\sigma^2(F_o^2) + (0.0388P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.70$ e Å^{-3}
$\Delta\rho_{min} = -0.67$ e Å^{-3}

Special details

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

	x	y	z	U_{iso}*/U_{eq}
Ag1	0.27879 (2)	1.03409 (3)	0.79027 (2)	0.05010 (9)
S1	0.26541 (6)	0.60865 (7)	0.78924 (5)	0.02831 (12)
O1	0.2153 (2)	0.7948 (2)	0.71897 (19)	0.0442 (4)
O2	0.1257 (2)	0.5487 (2)	0.87280 (17)	0.0403 (4)
O3	0.40789 (19)	0.5352 (2)	0.87452 (17)	0.0394 (4)
N1	0.0163 (2)	1.1487 (3)	0.8293 (2)	0.0375 (5)
N2	−0.2347 (3)	1.2925 (3)	0.9009 (2)	0.0432 (5)
H2A	−0.3130	1.3607	0.9392	0.052*
N3	0.5433 (3)	0.9312 (3)	0.7528 (2)	0.0452 (5)
N4	0.8038 (3)	0.7606 (3)	0.7855 (3)	0.0526 (6)
H4A	0.8907	0.6797	0.8272	0.063*
C1	−0.0695 (3)	1.2583 (3)	0.8957 (3)	0.0400 (6)

H1A	−0.0211	1.3053	0.9338	0.048*
C2	−0.2576 (3)	1.2010 (4)	0.8351 (3)	0.0478 (6)
H2B	−0.3600	1.1994	0.8230	0.057*
C3	−0.1029 (3)	1.1132 (3)	0.7907 (3)	0.0441 (6)
H3A	−0.0801	1.0397	0.7415	0.053*
C4	0.6465 (4)	0.8000 (4)	0.8461 (3)	0.0521 (7)
H4B	0.6136	0.7427	0.9413	0.063*
C5	0.8032 (3)	0.8703 (4)	0.6468 (3)	0.0500 (7)
H5A	0.8953	0.8729	0.5783	0.060*
C6	0.6423 (3)	0.9747 (4)	0.6280 (3)	0.0454 (6)
H6A	0.6041	1.0637	0.5423	0.054*
C7	0.3281 (2)	0.5262 (3)	0.6470 (2)	0.0261 (4)
C8	0.2202 (3)	0.4654 (3)	0.6223 (2)	0.0315 (5)
H8A	0.1202	0.4645	0.6810	0.038*
C9	0.2585 (3)	0.4046 (3)	0.5098 (3)	0.0356 (5)
H9A	0.1838	0.3637	0.4942	0.043*
C10	0.4037 (3)	0.4044 (3)	0.4227 (2)	0.0303 (5)
H10A	0.4281	0.3617	0.3492	0.036*
C11	0.5190 (2)	0.4687 (3)	0.4427 (2)	0.0244 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.02873 (11)	0.04781 (14)	0.06505 (16)	−0.00509 (8)	−0.00059 (8)	−0.02144 (11)
S1	0.0227 (2)	0.0346 (3)	0.0263 (3)	−0.0032 (2)	0.00093 (19)	−0.0173 (2)
O1	0.0487 (10)	0.0341 (9)	0.0476 (10)	−0.0029 (8)	−0.0031 (8)	−0.0236 (8)
O2	0.0293 (8)	0.0570 (11)	0.0346 (8)	−0.0124 (8)	0.0063 (7)	−0.0233 (8)
O3	0.0279 (8)	0.0556 (11)	0.0329 (8)	−0.0057 (7)	−0.0030 (6)	−0.0220 (8)
N1	0.0316 (10)	0.0353 (11)	0.0465 (11)	−0.0088 (8)	0.0017 (8)	−0.0205 (9)
N2	0.0362 (11)	0.0375 (11)	0.0476 (12)	−0.0032 (9)	0.0050 (9)	−0.0208 (10)
N3	0.0304 (11)	0.0365 (11)	0.0600 (14)	−0.0080 (9)	−0.0059 (10)	−0.0113 (10)
N4	0.0325 (11)	0.0442 (13)	0.0836 (18)	−0.0012 (9)	−0.0170 (11)	−0.0300 (13)
C1	0.0413 (13)	0.0409 (14)	0.0435 (13)	−0.0144 (11)	0.0025 (10)	−0.0232 (11)
C2	0.0337 (13)	0.0473 (15)	0.0614 (17)	−0.0097 (11)	−0.0081 (12)	−0.0203 (14)
C3	0.0415 (14)	0.0414 (14)	0.0579 (16)	−0.0109 (11)	−0.0037 (12)	−0.0291 (13)
C4	0.0435 (15)	0.0431 (15)	0.0591 (17)	−0.0119 (12)	−0.0076 (13)	−0.0094 (13)
C5	0.0403 (15)	0.0558 (17)	0.0661 (18)	−0.0174 (13)	0.0001 (13)	−0.0347 (16)
C6	0.0423 (14)	0.0419 (14)	0.0541 (16)	−0.0138 (12)	−0.0073 (12)	−0.0180 (13)
C7	0.0245 (10)	0.0275 (10)	0.0249 (10)	−0.0054 (8)	0.0001 (8)	−0.0126 (9)
C8	0.0260 (11)	0.0363 (12)	0.0346 (11)	−0.0126 (9)	0.0048 (9)	−0.0168 (10)
C9	0.0311 (12)	0.0424 (13)	0.0433 (13)	−0.0167 (10)	−0.0003 (9)	−0.0223 (11)
C10	0.0303 (11)	0.0349 (12)	0.0317 (11)	−0.0123 (9)	0.0006 (9)	−0.0182 (10)
C11	0.0252 (10)	0.0225 (10)	0.0236 (10)	−0.0051 (8)	−0.0016 (8)	−0.0095 (8)

Geometric parameters (Å, º)

Ag1—N1	2.1092 (19)	C2—C3	1.342 (4)
Ag1—N3	2.110 (2)	C2—H2B	0.9300

Ag1—O1	2.8180 (19)	C3—H3A	0.9300
S1—O1	1.4451 (19)	C4—H4B	0.9300
S1—O3	1.4511 (16)	C5—C6	1.343 (4)
S1—O2	1.4573 (18)	C5—H5A	0.9300
S1—C7	1.787 (2)	C6—H6A	0.9300
N1—C1	1.318 (3)	C7—C8	1.367 (3)
N1—C3	1.371 (3)	C7—C11^{i}	1.426 (3)
N2—C1	1.329 (3)	C8—C9	1.396 (3)
N2—C2	1.354 (4)	C8—H8A	0.9300
N2—H2A	0.8600	C9—C10	1.358 (3)
N3—C4	1.318 (3)	C9—H9A	0.9300
N3—C6	1.361 (4)	C10—C11	1.423 (3)
N4—C4	1.330 (4)	C10—H10A	0.9300
N4—C5	1.351 (4)	C11—C7^{i}	1.426 (3)
N4—H4A	0.8600	C11—C11^{i}	1.428 (4)
C1—H1A	0.9300		

N1—Ag1—N3	176.72 (8)	C2—C3—N1	109.5 (2)
N1—Ag1—O1	89.09 (7)	C2—C3—H3A	125.2
N3—Ag1—O1	94.16 (7)	N1—C3—H3A	125.2
O1—S1—O3	113.46 (11)	N3—C4—N4	110.8 (3)
O1—S1—O2	113.10 (11)	N3—C4—H4B	124.6
O3—S1—O2	111.15 (10)	N4—C4—H4B	124.6
O1—S1—C7	105.46 (10)	C6—C5—N4	105.9 (3)
O3—S1—C7	107.98 (9)	C6—C5—H5A	127.0
O2—S1—C7	105.03 (10)	N4—C5—H5A	127.0
S1—O1—Ag1	128.71 (10)	C5—C6—N3	110.0 (3)
C1—N1—C3	105.4 (2)	C5—C6—H6A	125.0
C1—N1—Ag1	130.79 (18)	N3—C6—H6A	125.0
C3—N1—Ag1	123.79 (16)	C8—C7—C11^{i}	120.85 (19)
C1—N2—C2	107.9 (2)	C8—C7—S1	117.59 (16)
C1—N2—H2A	126.1	C11^{i}—C7—S1	121.48 (16)
C2—N2—H2A	126.1	C7—C8—C9	120.6 (2)
C4—N3—C6	105.3 (2)	C7—C8—H8A	119.7
C4—N3—Ag1	126.0 (2)	C9—C8—H8A	119.7
C6—N3—Ag1	128.55 (18)	C10—C9—C8	120.8 (2)
C4—N4—C5	108.0 (2)	C10—C9—H9A	119.6
C4—N4—H4A	126.0	C8—C9—H9A	119.6
C5—N4—H4A	126.0	C9—C10—C11	120.8 (2)
N1—C1—N2	110.9 (2)	C9—C10—H10A	119.6
N1—C1—H1A	124.5	C11—C10—H10A	119.6
N2—C1—H1A	124.5	C10—C11—C7^{i}	123.01 (18)
C3—C2—N2	106.3 (2)	C10—C11—C11^{i}	118.9 (2)
C3—C2—H2B	126.8	C7^{i}—C11—C11^{i}	118.1 (2)
N2—C2—H2B	126.8		

O3—S1—O1—Ag1	−21.44 (16)	C5—N4—C4—N3	−0.2 (3)
O2—S1—O1—Ag1	106.34 (13)	C4—N4—C5—C6	0.2 (3)

C7—S1—O1—Ag1	−139.42 (11)	N4—C5—C6—N3	−0.1 (3)
N1—Ag1—O1—S1	−117.49 (14)	C4—N3—C6—C5	0.0 (3)
N3—Ag1—O1—S1	62.94 (14)	Ag1—N3—C6—C5	−175.65 (19)
O1—Ag1—N1—C1	165.5 (2)	O1—S1—C7—C8	−105.14 (19)
O1—Ag1—N1—C3	−11.9 (2)	O3—S1—C7—C8	133.26 (18)
O1—Ag1—N3—C4	−85.4 (2)	O2—S1—C7—C8	14.6 (2)
O1—Ag1—N3—C6	89.4 (2)	O1—S1—C7—C11^{i}	71.72 (19)
C3—N1—C1—N2	0.1 (3)	O3—S1—C7—C11^{i}	−49.88 (19)
Ag1—N1—C1—N2	−177.57 (16)	O2—S1—C7—C11^{i}	−168.56 (16)
C2—N2—C1—N1	0.1 (3)	C11^{i}—C7—C8—C9	0.9 (3)
C1—N2—C2—C3	−0.3 (3)	S1—C7—C8—C9	177.80 (18)
N2—C2—C3—N1	0.4 (3)	C7—C8—C9—C10	0.1 (4)
C1—N1—C3—C2	−0.3 (3)	C8—C9—C10—C11	−1.0 (4)
Ag1—N1—C3—C2	177.61 (18)	C9—C10—C11—C7^{i}	−179.0 (2)
C6—N3—C4—N4	0.1 (3)	C9—C10—C11—C11^{i}	0.9 (4)
Ag1—N3—C4—N4	175.93 (19)		

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4*A*···O2^{ii}	0.86	1.96	2.786 (3)	161
N2—H2*A*···O3^{iii}	0.86	2.37	2.998 (3)	130
N2—H2*A*···O3^{iv}	0.86	2.32	3.082 (3)	149

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