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Bis[μ-2-(3-pyridyl)-1*H*-benzimidazole-κ^2N:N']disilver(I) dinitrate

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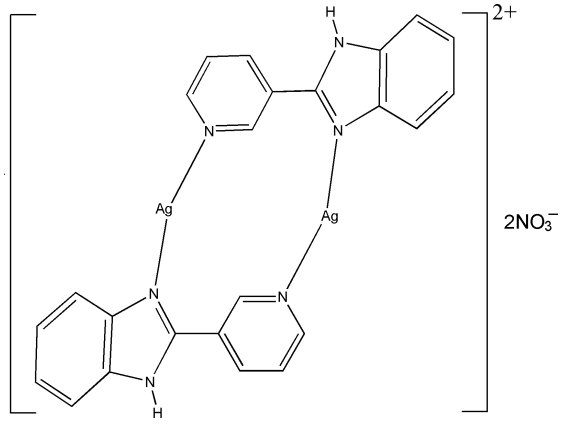
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.023; wR factor = 0.063; data-to-parameter ratio = 15.2.

The title compound, $[Ag_2(C_{12}H_9N_3)_2](NO_3)_2$, was prepared under hydrothermal conditions. The structure consists of binuclear complex cations and nitrate anions. The two Ag^I atoms, each in a geometry somewhat distorted from linear, are bridged by two 2-(3-pyridyl)benzimidazole ligands *via* pyridyl and imidazole N atoms, forming a centrosymmetric cyclic dimer. A three-dimensional network is constructed *via* N—H···O hydrogen bonds and weak Ag···O interactions [Ag···O = 2.686 (13)–2.847 (7) Å], as well as by offset π–π interactions between the pyridyl and imidazolyl rings with a nearest atom-to-atom distance of 3.40 (2) Å and a centroid-to-centroid distance of 4.06 (3) Å.

Related literature

For related literature, see: Alcade *et al.* (1992); Chen *et al.* (2005); Su *et al.* (1999).



Experimental

Crystal data

$[Ag_2(C_{12}H_9N_3)_2](NO_3)_2$
M_r = 730.20
Triclinic, $P\overline{1}$
a = 8.317 (3) Å
b = 9.097 (4) Å
c = 9.934 (4) Å
α = 105.949 (18)°
β = 96.797 (15)°
γ = 116.892 (11)°
V = 618.2 (5) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.64 mm^{-1}
T = 293 (2) K
0.50 × 0.45 × 0.40 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2000)
T_{min} = 0.444, T_{max} = 0.528
4673 measured reflections
2758 independent reflections
2586 reflections with $I > 2\sigma(I)$
R_{int} = 0.013

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.063
S = 1.04
2758 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.63 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—N2	2.1650 (19)	Ag1—N1^{i}	2.1994 (19)
N2—Ag1—N1^{i}	154.25 (7)		

Symmetry code: (i) $-x+2, -y+2, -z+2$.

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3B···O1^{ii}	0.86	2.01	2.860 (3)	172

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

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1994); 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: HY2089).

References

Alcade, E., Dinares, I., Perez-Garia, L. & Roca, T. (1992). *Synthesis*, pp. 295–398.
Chen, L. J., Xia, C. K., Zhang, Q. Z., Yang, W. B. & Lu, C. Z. (2005). *Inorg. Chem. Commun.* **8**, 858–861.
Rigaku (2000). *CrystalClear*. Version 1.35. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Siemens (1994). *SHELXTL*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Su, C. Y., Yang, X. P., Liao, S., Mak, T. C. W. & Kang, B. S. (1999). *Inorg. Chem. Commun.* **2**, 383–385.

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supplementary materials

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Bis[μ-2-(3-pyridyl)-1*H*-benzimidazole-κ^2N:*N*']disilver(I) dinitrate

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Comment

The 2-(3-pyridyl)benzimidazole ligand acts as terminal (Chen *et al.*, 2005) or bidentate ligand (Su *et al.*, 1999) in metal complexes. Herein we report the synthesis and structure of a binuclear silver(I) complex with 2-(3-pyridyl)benzimidazole.

In the title compound, the centrosymmetric binuclear cyclic complex contains two Ag^I atoms bridged by two 2-(3-pyridyl)benzimidazole ligands *via* pyridyl and imidazole N atoms in a head-to-end mode (Fig. 1). The Ag^I atom is in an approximate linear coordination geometry. The nitrate anion acts as a counter ion and is weakly coordinated to Ag^I atoms [Ag1···O1 = 2.686 (13) Å, Ag1···O3 = 2.847 (7)Å and Ag1···O2^i = 2.782 (5) Å; symmetry code: (i) $1-x, 2-y, 2-z$]. The Ag1···O1 and Ag1···O3 interactions as well as N3—H···O1 hydrogen bonds connect the binuclear units into a one-dimensional chain (Fig. 2). Crystal packing is stabilized by the Ag1···O2^i interactions and offset π–π interactions between the chains (Fig. 3).

Experimental

A solution of $AgNO_3$ (0.104 g, 0.61 mmol), 2-(3-pyridyl)benzimidazole (Alcade *et al.*, 1992) (0.14 g, 0.61 mmol) and H_2O (15 ml) was stirred under ambient condition. The mixture was sealed in a 25 ml Teflon-lined stainless steel vessel, heated at 383 K for 3 d and then cooled to room temperature. The resulting product was collected by filtration, washed with distilled water and dried in air (yield 80%).

Refinement

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 and N—H = 0.86Å and U_{iso}(H) = 1.2U_{eq}(C,*N*).

Figures

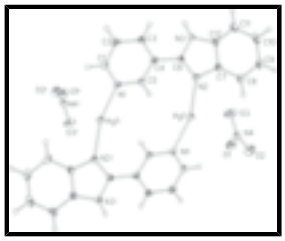


Fig. 1. The structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) $2-x, 2-y, 2-z$.]

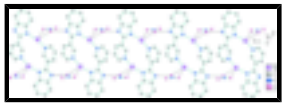


Fig. 2. A view of the one-dimensional chain. H atoms have been omitted for clarity. Hydrogen bonds and weak Ag···O interactions are shown as dashed lines.

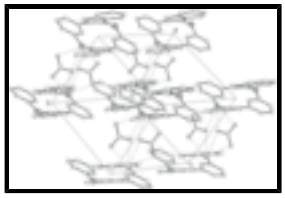


Fig. 3. The crystal packing of the title compound. Hydrogen bonds and weak Ag···O interactions are shown as dashed lines.

Bis[μ-2-(3-pyridyl)-1*H*-benzimidazole-κ^2N:*N*']disilver(I) dinitrate

Crystal data

$[Ag_2(C_{12}H_9N_3)_2](NO_3)_2$	$Z = 1$
$M_r = 730.20$	$F_{000} = 360$
Triclinic, $P\overline{1}$	$D_x = 1.962$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.317$ (3) Å	Cell parameters from 1908 reflections
$b = 9.097$ (4) Å	$\theta = 2.7$–27.5º
$c = 9.934$ (4) Å	$\mu = 1.64$ mm^{-1}
$\alpha = 105.949$ (18)º	$T = 293$ (2) K
$\beta = 96.797$ (15)º	Prism, colorless
$\gamma = 116.892$ (11)º	0.50 × 0.45 × 0.40 mm
$V = 618.2$ (5) Å^3	

Data collection

Rigaku Mercury CCD diffractometer	2758 independent reflections
Radiation source: fine-focus sealed tube	2586 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.013$
$T = 293$(2) K	$\theta_{max} = 27.5$º
ω scans	$\theta_{min} = 2.7$º
Absorption correction: multi-scan (CrystalClear; Rigaku, 2000)	$h = -10\rightarrow6$
$T_{min} = 0.444$, $T_{max} = 0.528$	$k = -10\rightarrow11$
4673 measured reflections	$l = -12\rightarrow12$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.024$	H-atom parameters constrained
$wR(F^2) = 0.063$	$w = 1/[\sigma^2(F_o^2) + (0.0396P)^2 + 0.1553P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.002$
2758 reflections	$\Delta\rho_{max} = 0.59$ e Å^{-3}

181 parameters	$\Delta\rho_{min} = -0.63$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ag1	0.69487 (2)	0.909984 (19)	0.836791 (18)	0.03879 (8)
C1	1.0525 (3)	0.7222 (3)	1.1866 (2)	0.0340 (4)
H1A	1.1496	0.7688	1.2706	0.041*
C2	0.8990 (3)	0.5561 (3)	1.1521 (2)	0.0349 (4)
H2A	0.8944	0.4912	1.2108	0.042*
C3	0.7521 (3)	0.4871 (3)	1.0294 (2)	0.0315 (4)
H3A	0.6471	0.3754	1.0046	0.038*
C4	0.7635 (3)	0.5871 (3)	0.9437 (2)	0.0275 (4)
C5	0.9260 (3)	0.7512 (3)	0.9839 (2)	0.0299 (4)
H5A	0.9368	0.8166	0.9246	0.036*
C6	0.6097 (3)	0.5236 (2)	0.8146 (2)	0.0278 (4)
C7	0.4068 (3)	0.5075 (3)	0.6448 (2)	0.0296 (4)
C8	0.2976 (3)	0.5400 (3)	0.5523 (2)	0.0377 (5)
H8A	0.3261	0.6549	0.5640	0.045*
C9	0.1461 (3)	0.3949 (4)	0.4431 (3)	0.0452 (5)
H9A	0.0698	0.4125	0.3809	0.054*
C10	0.1036 (3)	0.2212 (4)	0.4230 (3)	0.0485 (6)
H10A	0.0002	0.1266	0.3476	0.058*
C11	0.2107 (3)	0.1873 (3)	0.5119 (3)	0.0420 (5)
H11A	0.1839	0.0722	0.4977	0.050*
C12	0.3621 (3)	0.3342 (3)	0.6251 (2)	0.0320 (4)
N1	1.0673 (2)	0.8195 (2)	1.10372 (19)	0.0310 (3)
N2	0.5635 (2)	0.6242 (2)	0.76462 (17)	0.0285 (3)
N3	0.4925 (2)	0.3486 (2)	0.73404 (19)	0.0323 (4)
H3B	0.4988	0.2622	0.7486	0.039*
N4	0.3636 (3)	0.9842 (2)	0.83250 (19)	0.0333 (4)
O1	0.4791 (3)	1.0384 (3)	0.7610 (2)	0.0500 (4)
O2	0.2846 (3)	1.0683 (3)	0.8762 (2)	0.0503 (4)
O3	0.3345 (3)	0.8520 (3)	0.8593 (2)	0.0623 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.03312 (11)	0.02520 (10)	0.05195 (12)	0.01146 (8)	0.00234 (8)	0.01578 (8)
C1	0.0334 (11)	0.0342 (11)	0.0355 (10)	0.0180 (9)	0.0048 (8)	0.0151 (8)
C2	0.0369 (11)	0.0375 (11)	0.0399 (10)	0.0203 (10)	0.0140 (9)	0.0240 (9)
C3	0.0300 (10)	0.0273 (10)	0.0393 (10)	0.0130 (8)	0.0126 (8)	0.0168 (8)
C4	0.0267 (9)	0.0252 (9)	0.0341 (9)	0.0148 (8)	0.0094 (8)	0.0128 (7)
C5	0.0273 (10)	0.0250 (9)	0.0389 (10)	0.0131 (8)	0.0064 (8)	0.0155 (8)
C6	0.0233 (9)	0.0231 (9)	0.0351 (9)	0.0087 (7)	0.0080 (7)	0.0137 (7)
C7	0.0245 (9)	0.0311 (10)	0.0333 (9)	0.0127 (8)	0.0092 (8)	0.0139 (8)

C8	0.0395 (12)	0.0449 (12)	0.0377 (10)	0.0259 (11)	0.0113 (9)	0.0197 (9)
C9	0.0361 (12)	0.0635 (16)	0.0377 (11)	0.0267 (12)	0.0061 (9)	0.0207 (11)
C10	0.0313 (12)	0.0538 (15)	0.0387 (11)	0.0104 (11)	0.0001 (9)	0.0109 (11)
C11	0.0337 (12)	0.0330 (11)	0.0432 (12)	0.0073 (10)	0.0050 (9)	0.0113 (9)
C12	0.0251 (9)	0.0311 (10)	0.0347 (10)	0.0097 (8)	0.0068 (8)	0.0140 (8)
N1	0.0268 (8)	0.0253 (8)	0.0401 (9)	0.0130 (7)	0.0047 (7)	0.0134 (7)
N2	0.0265 (8)	0.0256 (8)	0.0342 (8)	0.0132 (7)	0.0074 (7)	0.0128 (6)
N3	0.0287 (9)	0.0229 (8)	0.0400 (9)	0.0092 (7)	0.0039 (7)	0.0135 (7)
N4	0.0293 (9)	0.0276 (9)	0.0381 (9)	0.0129 (7)	0.0011 (7)	0.0117 (7)
O1	0.0481 (10)	0.0499 (10)	0.0734 (12)	0.0307 (9)	0.0297 (9)	0.0373 (9)
O2	0.0553 (11)	0.0530 (11)	0.0576 (10)	0.0381 (10)	0.0188 (9)	0.0214 (9)
O3	0.0801 (15)	0.0443 (10)	0.0842 (14)	0.0360 (11)	0.0334 (12)	0.0418 (10)

Geometric parameters (Å, °)

Ag1—N2	2.1650 (19)	C7—C8	1.396 (3)
Ag1—N1^{i}	2.1994 (19)	C8—C9	1.375 (3)
C1—N1	1.343 (3)	C8—H8A	0.9300
C1—C2	1.377 (3)	C9—C10	1.403 (4)
C1—H1A	0.9300	C9—H9A	0.9300
C2—C3	1.381 (3)	C10—C11	1.371 (4)
C2—H2A	0.9300	C10—H10A	0.9300
C3—C4	1.389 (3)	C11—C12	1.397 (3)
C3—H3A	0.9300	C11—H11A	0.9300
C4—C5	1.391 (3)	C12—N3	1.372 (3)
C4—C6	1.467 (3)	N1—Ag1^{i}	2.1994 (19)
C5—N1	1.336 (3)	N3—O1^{ii}	2.860 (3)
C5—H5A	0.9300	N3—H3B	0.8600
C6—N2	1.324 (2)	N4—O3	1.226 (3)
C6—N3	1.355 (3)	N4—O2	1.243 (2)
C7—N2	1.389 (3)	N4—O1	1.263 (3)
C7—C12	1.395 (3)		
N2—Ag1—N1^{i}	154.25 (7)	C8—C9—H9A	119.1
N1—C1—C2	122.6 (2)	C10—C9—H9A	119.1
N1—C1—H1A	118.7	C11—C10—C9	121.6 (2)
C2—C1—H1A	118.7	C11—C10—H10A	119.2
C1—C2—C3	119.25 (19)	C9—C10—H10A	119.2
C1—C2—H2A	120.4	C10—C11—C12	116.6 (2)
C3—C2—H2A	120.4	C10—C11—H11A	121.7
C2—C3—C4	119.00 (19)	C12—C11—H11A	121.7
C2—C3—H3A	120.5	N3—C12—C7	105.85 (18)
C4—C3—H3A	120.5	N3—C12—C11	132.0 (2)
C3—C4—C5	118.03 (19)	C7—C12—C11	122.1 (2)
C3—C4—C6	121.62 (18)	C5—N1—C1	118.00 (18)
C5—C4—C6	120.35 (17)	C5—N1—Ag1^{i}	119.02 (13)
N1—C5—C4	123.10 (18)	C1—N1—Ag1^{i}	122.89 (14)
N1—C5—H5A	118.4	C6—N2—C7	105.76 (16)
C4—C5—H5A	118.4	C6—N2—Ag1	130.80 (14)

N2—C6—N3	111.85 (18)	C7—N2—Ag1	123.40 (13)
N2—C6—C4	125.91 (18)	C6—N3—C12	107.64 (17)
N3—C6—C4	122.21 (18)	C6—N3—O1^{ii}	131.71 (14)
N2—C7—C12	108.90 (17)	C12—N3—O1^{ii}	120.65 (14)
N2—C7—C8	130.6 (2)	C6—N3—H3B	126.2
C12—C7—C8	120.5 (2)	C12—N3—H3B	126.2
C9—C8—C7	117.2 (2)	O3—N4—O2	121.6 (2)
C9—C8—H8A	121.4	O3—N4—O1	119.38 (19)
C7—C8—H8A	121.4	O2—N4—O1	119.00 (19)
C8—C9—C10	121.9 (2)		
N1—C1—C2—C3	−1.4 (3)	C4—C5—N1—Ag1^{i}	−174.98 (14)
C1—C2—C3—C4	0.3 (3)	C2—C1—N1—C5	0.5 (3)
C2—C3—C4—C5	1.6 (3)	C2—C1—N1—Ag1^{i}	176.94 (16)
C2—C3—C4—C6	−178.09 (18)	N3—C6—N2—C7	0.1 (2)
C3—C4—C5—N1	−2.7 (3)	C4—C6—N2—C7	−177.85 (18)
C6—C4—C5—N1	177.04 (18)	N3—C6—N2—Ag1	−177.81 (12)
C3—C4—C6—N2	148.1 (2)	C4—C6—N2—Ag1	4.2 (3)
C5—C4—C6—N2	−31.7 (3)	C12—C7—N2—C6	−0.2 (2)
C3—C4—C6—N3	−29.7 (3)	C8—C7—N2—C6	178.7 (2)
C5—C4—C6—N3	150.54 (19)	C12—C7—N2—Ag1	177.91 (13)
N2—C7—C8—C9	−178.6 (2)	C8—C7—N2—Ag1	−3.2 (3)
C12—C7—C8—C9	0.2 (3)	N1^{i}—Ag1—N2—C6	52.9 (2)
C7—C8—C9—C10	−1.0 (3)	N1^{i}—Ag1—N2—C7	−124.70 (17)
C8—C9—C10—C11	0.3 (4)	N2—C6—N3—C12	0.0 (2)
C9—C10—C11—C12	1.1 (4)	C4—C6—N3—C12	178.08 (17)
N2—C7—C12—N3	0.2 (2)	N2—C6—N3—O1^{ii}	−178.99 (13)
C8—C7—C12—N3	−178.82 (18)	C4—C6—N3—O1^{ii}	−0.9 (3)
N2—C7—C12—C11	−179.67 (19)	C7—C12—N3—C6	−0.2 (2)
C8—C7—C12—C11	1.3 (3)	C11—C12—N3—C6	179.7 (2)
C10—C11—C12—N3	178.2 (2)	C7—C12—N3—O1^{ii}	178.99 (12)
C10—C11—C12—C7	−1.9 (3)	C11—C12—N3—O1^{ii}	−1.1 (3)
C4—C5—N1—C1	1.6 (3)		

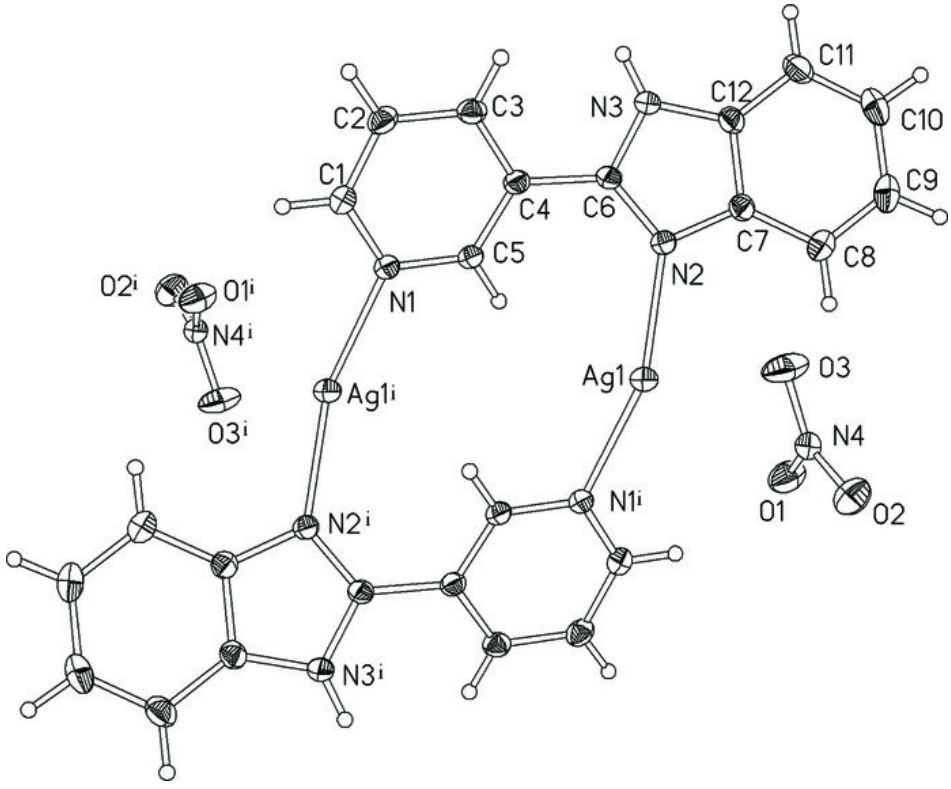
Symmetry codes: (i) −*x*+2, −*y*+2, −*z*+2; (ii) *x*, *y*−1, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3B···O1^{ii}	0.86	2.01	2.860 (3)	172

Symmetry codes: (ii) *x*, *y*−1, *z*.

Fig. 1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C12
N3
C10
C2
C3
C9
C1
C4
C6
C7
C8
C5
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N3i

Fig. 2

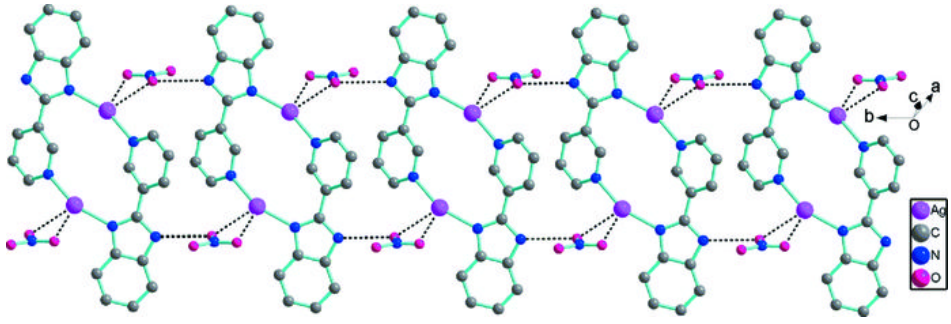

Fig. 3