Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(2,2′-Bipyridyl-κ^2N,N')(succinamidato-κN)silver(I)

David R. Whitcomb[a] and Manju Rajeswaran[b]*

[a]Carestream Health, Inc., 1 Imation Way, Oakdale, MN 55129, USA, and [b]Eastman Kodak Company, Kodak Research Laboratories, Rochester, NY 14650-2106, USA
Correspondence e-mail: manju.rajeswaran@kodak.com

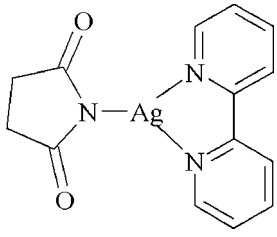
Received 8 October 2007; accepted 13 October 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.037; wR factor = 0.084; data-to-parameter ratio = 16.4.

In the molecular title complex, $[Ag(C_4H_4NO_2)(C_{10}H_8N_2)]$, the Ag atom adopts a distorted T-shaped AgN_3 coordination. Aromatic π–π stacking interactions [centroid–centroid separation = 3.8393 (17) Å] lead to centrosymmetric dimers of molecules in the crystal structure.

Related literature

For related literature, see: Fijolek *et al.* (1997); Jaber *et al.* (1996); Oldham & Sandford (1977); Othman *et al.* (2003); Tolochko *et al.* (1998); Voicu *et al.* (2001); Whitcomb & Rajeswaran (2006*a*,*b*,*c*).



Experimental

Crystal data

$[Ag(C_4H_4NO_2)(C_{10}H_8N_2)]$
M_r = 362.14
Monoclinic, $P2_1/n$
a = 12.0853 (3) Å
b = 7.4188 (2) Å
c = 14.6724 (4) Å
β = 99.924 (1)°
V = 1295.82 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.56 mm^{-1}
T = 293 (2) K
0.5 × 0.25 × 0.15 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SORTAV*; Blessing 1995)
T_{min} = 0.706, T_{max} = 0.871
(expected range = 0.641–0.791)
14369 measured reflections
2967 independent reflections
2176 reflections with $I > 2\sigma(I)$
R_{int} = 0.069

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.084
S = 1.07
2967 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.98 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—N1	2.108 (2)	Ag1—N3	2.422 (2)
Ag1—N2	2.225 (2)		
N1—Ag1—N2	168.37 (9)	N2—Ag1—N3	71.30 (8)
N1—Ag1—N3	120.30 (8)		

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXTL* (Bruker, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* and *Materials Studio* (Accelrys, 2002); software used to prepare material for publication: *publCIF* (Westrip, 2007).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2575).

References

Accelrys (2002). *Materials Studio*. Version 2.2.1. Accelrys Inc., San Diego, California, USA.
Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Bruker (2001). *SHELXTL*. Version 6.12. Bruker AXS Inc., Madison, Wisconsin, USA.
Fijolek, H. G., González, P., Park, S. H., Suib, S. L. & Natan, M. J. (1997). *Inorg. Chem.* **36**, 5299–5305.
Jaber, F., Charbonnier, F., Petit-Ramel, M. & Faure, R. (1996). *Eur. J. Solid State Inorg. Chem.* **33**, 429–440.
Nonius (2000). *COLLECT*. Nonius BV, Delft, The Netherlands.
Oldham, C. & Sandford, W. F. (1977). *J. Chem. Soc. Dalton Trans.* pp. 2068–2070.
Othman, B., Effendy, A. H., Skelton, B. W. & White, A. H. (2003). *Aust. J. Chem.* **56**, 719–721.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Tolochko, B. P., Chernov, S. V., Nikitenko, S. G. & Whitcomb, D. R. (1998). *Nucl. Instrum. Methods Phys. Res. A*, **405**, 428–434.
Voicu, R., Badia, A., Morin, F., Lennox, R. B. & Ellis, T. H. (2001). *Chem. Mater.* **13**, 2266–2271.
Whitcomb, D. R. & Rajeswaran, M. (2006*a*). *Polyhedron*, **25**, 1747–1752.
Whitcomb, D. R. & Rajeswaran, M. (2006*b*). *J. Chem. Crystallogr.* **36**, 587–598.
Whitcomb, D. R. & Rajeswaran, M. (2006*c*). *Acta Cryst.* E**62**, m272–m274.
Westrip, S. P. (2006). *publCIF*. In preparation.

 doi:10.1107/S1600536807050301

supplementary materials

Acta Cryst. (2007). E**63**, m2753 [**doi:10.1107/S1600536807050301**]

(2,2'-Bipyridyl-κ^2N,N')(succinamidato-κN)silver(I)

D. R. Whitcomb and M. Rajeswaran

Comment

Most homoleptic silver coordination complexes form polymeric structures, many of which exhibit poor solubility, such as silver carboxylates (Tolochko *et al.*, 1998; Whitcomb and Rajeswaran, 2006*a;* Jaber *et al.*, 1996), silver cyclic amidates (Whitcomb and Rajeswaran 2006*b;* Whitcomb and Rajeswaran, 2006*c*), and silver thiolates (Fijolek *et al.*, 1997; Voicu *et al.*, 2001). The connecting groups of these polymeric structures can be disrupted by incorporating argentophilic neutral-donor ligands into the complex, especially triarylphosphines (Oldham and Sandford, 1977; Othman *et al.*, 2003; Whitcomb and Rajeswaran, 2006*b*). In our investigations to manipulate the solid-state structure of silver complexes, we now consider the effect of weaker argentophilic N donor atoms in the ligand 2,2'-dipyridyl (dipy, $C_{10}H_8N_2$). We report here the crystal structure of the title silver complex, (I).

The new structure is a simple molecular complex of both ligands, having the composition AgSI-dipy (SI = succinimide anion, $C_4H_4NO_2^-$), which are additionally held together by π-π stacking interactions between dipy rings with centroid separations of 3.8393 (17) Å. The molecular structure of (I) is shown in Fig. 1, and the packing diagram of the π-π -bonded dimers is given in Fig 2. In order to achieve this structure, the dipy ligand both depolymerized and dehydrated the starting $\{[AgSI]_2{\cdot}H_2O\}$ complex.

The structures of three complexes of silver cyclic amides can now be compared: the title complex, the starting $\{[AgSI]_2{\cdot}H_2O\}$ complex (Whitcomb and Rajeswaran, 2006*c*), and the related bis-triphenylphosphine silver phthalimide (Whitcomb and Rajeswaran, 2006*b*). The starting $\{[AgSI]_2{\cdot}H_2O\}$ complex exhibits the shortest Ag—N bond lengths at 2.077 (3) and 2.095 (3) Å, while the phthalimide complex has a single Ag—N at 2.223 (3) Å. The Ag—N bonds of the title complex (Table 1) span the normal range with a tendency to the high side.

Experimental

Silver succinate hydrate (Whitcomb and Rajeswaran, 2006*c*) (0.40 g) was reacted with 0.40 g bipyridyl in 20 ml EtOH. The thick dispersion completely cleared with mild heating. Slow cooling yielded colourless rods of (I). M·P. 454 K (sharp). Analysis: calc. for $C_{14}H_{12}N_3O_2Ag$: C = 46.43, H =3.34, N =11.60%, found C = 46.15, H =3.15, N =11.31%.

Figures

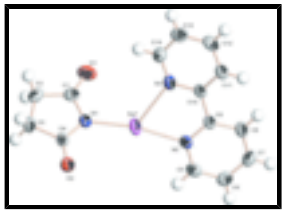


Fig. 1. The molecular structure of (I) with 50% probability displacement ellipsoids for non-hydrogen atoms.

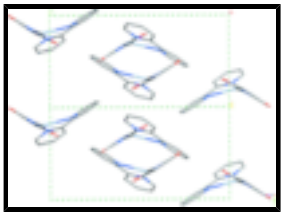


Fig. 2. Packing diagram for (I).

(2,2'-Bipyidyl-κ^2*N*,*N*')(succinamidato-κ*N*)silver

Crystal data

$[Ag(C_4H_4NO_2)(C_{10}H_8N_2)]$	F_{000} = 720
M_r = 362.14	D_x = 1.856 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 8777 reflections
a = 12.0853 (3) Å	θ = 1.0–27.5º
b = 7.4188 (2) Å	μ = 1.56 mm^{-1}
c = 14.6724 (4) Å	T = 293 (2) K
β = 99.924 (1)º	Rod, colorless
V = 1295.82 (6) Å^3	0.5 × 0.25 × 0.15 mm
Z = 4	

Data collection

Nonius KappaCCD diffractometer	2967 independent reflections
Radiation source: fine-focus sealed tube	2176 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.069
Detector resolution: 9 pixels mm^{-1}	θ_{max} = 27.5º
T = 293(2) K	θ_{min} = 4.1º
ω and φ scans	h = −15→15
Absorption correction: multi-scan (SORTAV; Blessing 1995)	k = −7→9
T_{min} = 0.706, T_{max} = 0.871	l = −16→19
14369 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.037	H-atom parameters constrained
$wR(F^2)$ = 0.084	$w = 1/[\sigma^2(F_o^2) + (0.0421P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.07	$(\Delta/\sigma)_{max}$ = 0.002
2967 reflections	$\Delta\rho_{max}$ = 0.44 e Å^{-3}

181 parameters	$\Delta\rho_{min} = -0.98$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ag1	0.180684 (16)	0.19961 (3)	1.040989 (15)	0.04664 (12)
O1	0.4046 (2)	0.3033 (3)	0.96269 (17)	0.0641 (7)
O2	0.36059 (15)	0.0042 (3)	1.22380 (13)	0.0497 (5)
N1	0.35406 (18)	0.1646 (3)	1.08880 (16)	0.0374 (6)
N2	−0.00208 (19)	0.2619 (3)	1.01848 (16)	0.0348 (5)
N3	0.09929 (18)	0.1201 (4)	0.88357 (16)	0.0403 (6)
C1	0.4306 (3)	0.2259 (4)	1.0372 (2)	0.0413 (7)
C2	0.5483 (3)	0.1835 (4)	1.0839 (2)	0.0448 (8)
H2A	0.5902	0.2931	1.1019	0.054*
H2B	0.5876	0.1140	1.0434	0.054*
C3	0.5330 (2)	0.0749 (4)	1.1676 (2)	0.0438 (7)
H3A	0.5720	0.1305	1.2239	0.053*
H3B	0.5607	−0.0470	1.1637	0.053*
C4	0.4069 (2)	0.0756 (4)	1.16514 (19)	0.0351 (6)
C5	−0.0482 (3)	0.3534 (4)	1.0814 (2)	0.0413 (7)
H5	−0.0037	0.3801	1.1380	0.050*
C6	−0.1581 (2)	0.4094 (4)	1.0658 (2)	0.0438 (7)
H6	−0.1871	0.4721	1.1113	0.053*
C7	−0.2248 (2)	0.3717 (5)	0.9821 (2)	0.0454 (7)
H7	−0.2993	0.4093	0.9699	0.054*
C8	−0.1789 (2)	0.2764 (4)	0.9162 (2)	0.0429 (7)
H8	−0.2224	0.2486	0.8593	0.051*
C9	−0.0668 (2)	0.2231 (4)	0.93656 (19)	0.0322 (6)
C10	−0.0127 (2)	0.1233 (4)	0.86720 (18)	0.0334 (6)
C11	−0.0747 (2)	0.0387 (4)	0.79043 (19)	0.0408 (7)
H11	−0.1528	0.0412	0.7802	0.049*
C12	−0.0174 (3)	−0.0496 (4)	0.7294 (2)	0.0468 (7)
H12	−0.0569	−0.1067	0.6774	0.056*
C13	0.0980 (3)	−0.0524 (4)	0.7463 (2)	0.0493 (8)
H13	0.1380	−0.1107	0.7061	0.059*

C14	0.1524 (2)	0.0329 (4)	0.8237 (2)	0.0474 (8)
H14	0.2305	0.0304	0.8355	0.057*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.03268 (15)	0.05414 (19)	0.04831 (18)	−0.00169 (10)	−0.00653 (10)	0.00760 (11)
O1	0.0784 (17)	0.0724 (17)	0.0437 (15)	0.0069 (12)	0.0170 (12)	0.0134 (12)
O2	0.0411 (11)	0.0646 (14)	0.0435 (12)	−0.0047 (11)	0.0074 (9)	0.0113 (11)
N1	0.0327 (12)	0.0456 (14)	0.0330 (13)	0.0016 (10)	0.0030 (10)	−0.0013 (11)
N2	0.0362 (12)	0.0354 (12)	0.0316 (13)	−0.0028 (10)	0.0028 (10)	0.0039 (10)
N3	0.0335 (12)	0.0463 (14)	0.0391 (14)	0.0004 (11)	0.0010 (10)	0.0017 (12)
C1	0.0476 (17)	0.0403 (17)	0.0384 (17)	0.0021 (14)	0.0139 (14)	−0.0046 (14)
C2	0.0398 (16)	0.0470 (19)	0.0507 (19)	−0.0045 (13)	0.0167 (14)	−0.0099 (14)
C3	0.0307 (14)	0.0497 (19)	0.0491 (18)	0.0007 (13)	0.0018 (12)	−0.0019 (14)
C4	0.0325 (13)	0.0357 (15)	0.0354 (15)	0.0010 (12)	0.0010 (11)	−0.0065 (13)
C5	0.0504 (18)	0.0396 (16)	0.0337 (16)	−0.0040 (14)	0.0061 (13)	0.0054 (13)
C6	0.0482 (17)	0.0409 (17)	0.0450 (18)	−0.0005 (14)	0.0159 (14)	0.0011 (14)
C7	0.0356 (15)	0.0464 (18)	0.056 (2)	0.0046 (14)	0.0129 (14)	0.0055 (16)
C8	0.0351 (15)	0.0493 (19)	0.0422 (17)	−0.0020 (13)	0.0007 (12)	0.0043 (15)
C9	0.0319 (14)	0.0297 (14)	0.0341 (15)	−0.0020 (11)	0.0030 (11)	0.0062 (12)
C10	0.0348 (14)	0.0317 (14)	0.0328 (15)	−0.0025 (12)	0.0031 (11)	0.0076 (12)
C11	0.0382 (15)	0.0427 (16)	0.0386 (16)	−0.0032 (13)	−0.0013 (12)	0.0033 (14)
C12	0.0576 (18)	0.0435 (18)	0.0364 (16)	−0.0037 (15)	0.0001 (13)	−0.0045 (14)
C13	0.0620 (19)	0.0455 (18)	0.0427 (18)	0.0083 (15)	0.0150 (15)	−0.0016 (14)
C14	0.0390 (16)	0.059 (2)	0.0446 (18)	0.0069 (14)	0.0085 (13)	0.0020 (15)

Geometric parameters (Å, °)

Ag1—N1	2.108 (2)	C5—C6	1.372 (4)
Ag1—N2	2.225 (2)	C5—H5	0.9300
Ag1—N3	2.422 (2)	C6—C7	1.377 (4)
O1—C1	1.227 (4)	C6—H6	0.9300
O2—C4	1.225 (3)	C7—C8	1.388 (5)
N1—C4	1.361 (4)	C7—H7	0.9300
N1—C1	1.369 (4)	C8—C9	1.393 (4)
N2—C5	1.342 (4)	C8—H8	0.9300
N2—C9	1.347 (3)	C9—C10	1.497 (4)
N3—C10	1.333 (3)	C10—C11	1.390 (4)
N3—C14	1.341 (4)	C11—C12	1.387 (4)
C1—C2	1.502 (4)	C11—H11	0.9300
C2—C3	1.507 (4)	C12—C13	1.374 (4)
C2—H2A	0.9700	C12—H12	0.9300
C2—H2B	0.9700	C13—C14	1.366 (4)
C3—C4	1.518 (3)	C13—H13	0.9300
C3—H3A	0.9700	C14—H14	0.9300
C3—H3B	0.9700		
N1—Ag1—N2	168.37 (9)	N2—C5—C6	122.9 (3)

N1—Ag1—N3	120.30 (8)	N2—C5—H5	118.5
N2—Ag1—N3	71.30 (8)	C6—C5—H5	118.5
C4—N1—C1	110.5 (2)	C5—C6—C7	119.2 (3)
C4—N1—Ag1	129.19 (18)	C5—C6—H6	120.4
C1—N1—Ag1	120.15 (19)	C7—C6—H6	120.4
C5—N2—C9	118.4 (2)	C6—C7—C8	118.8 (3)
C5—N2—Ag1	121.49 (19)	C6—C7—H7	120.6
C9—N2—Ag1	119.80 (18)	C8—C7—H7	120.6
C10—N3—C14	118.5 (3)	C7—C8—C9	119.1 (3)
C10—N3—Ag1	113.59 (17)	C7—C8—H8	120.5
C14—N3—Ag1	125.51 (18)	C9—C8—H8	120.5
O1—C1—N1	123.7 (3)	N2—C9—C8	121.6 (3)
O1—C1—C2	125.5 (3)	N2—C9—C10	117.2 (2)
N1—C1—C2	110.8 (3)	C8—C9—C10	121.2 (3)
C1—C2—C3	104.1 (2)	N3—C10—C11	121.7 (3)
C1—C2—H2A	110.9	N3—C10—C9	115.8 (2)
C3—C2—H2A	110.9	C11—C10—C9	122.5 (2)
C1—C2—H2B	110.9	C12—C11—C10	118.5 (3)
C3—C2—H2B	110.9	C12—C11—H11	120.8
H2A—C2—H2B	109.0	C10—C11—H11	120.8
C2—C3—C4	104.0 (2)	C13—C12—C11	119.7 (3)
C2—C3—H3A	111.0	C13—C12—H12	120.2
C4—C3—H3A	111.0	C11—C12—H12	120.2
C2—C3—H3B	111.0	C14—C13—C12	118.1 (3)
C4—C3—H3B	111.0	C14—C13—H13	121.0
H3A—C3—H3B	109.0	C12—C13—H13	121.0
O2—C4—N1	125.6 (2)	N3—C14—C13	123.5 (3)
O2—C4—C3	124.0 (3)	N3—C14—H14	118.2
N1—C4—C3	110.3 (2)	C13—C14—H14	118.2
N2—Ag1—N1—C4	57.8 (5)	Ag1—N2—C5—C6	173.4 (2)
N3—Ag1—N1—C4	−127.1 (2)	N2—C5—C6—C7	−0.3 (4)
N2—Ag1—N1—C1	−126.9 (4)	C5—C6—C7—C8	0.6 (4)
N3—Ag1—N1—C1	48.2 (2)	C6—C7—C8—C9	−0.4 (5)
N1—Ag1—N2—C5	4.4 (5)	C5—N2—C9—C8	0.3 (4)
N3—Ag1—N2—C5	−171.1 (2)	Ag1—N2—C9—C8	−173.3 (2)
N1—Ag1—N2—C9	177.9 (4)	C5—N2—C9—C10	179.1 (2)
N3—Ag1—N2—C9	2.36 (19)	Ag1—N2—C9—C10	5.4 (3)
N1—Ag1—N3—C10	170.39 (19)	C7—C8—C9—N2	−0.1 (4)
N2—Ag1—N3—C10	−10.66 (19)	C7—C8—C9—C10	−178.8 (3)
N1—Ag1—N3—C14	8.5 (3)	C14—N3—C10—C11	0.2 (4)
N2—Ag1—N3—C14	−172.5 (3)	Ag1—N3—C10—C11	−163.0 (2)
C4—N1—C1—O1	176.5 (3)	C14—N3—C10—C9	−179.9 (2)
Ag1—N1—C1—O1	0.4 (4)	Ag1—N3—C10—C9	16.8 (3)
C4—N1—C1—C2	−2.9 (3)	N2—C9—C10—N3	−15.5 (4)
Ag1—N1—C1—C2	−179.00 (18)	C8—C9—C10—N3	163.2 (3)
O1—C1—C2—C3	−175.1 (3)	N2—C9—C10—C11	164.4 (3)
N1—C1—C2—C3	4.2 (3)	C8—C9—C10—C11	−16.9 (4)
C1—C2—C3—C4	−3.8 (3)	N3—C10—C11—C12	−0.6 (4)
C1—N1—C4—O2	−179.2 (3)	C9—C10—C11—C12	179.6 (3)

Ag1—N1—C4—O2	−3.6 (4)	C10—C11—C12—C13	0.4 (4)
C1—N1—C4—C3	0.3 (3)	C11—C12—C13—C14	0.1 (5)
Ag1—N1—C4—C3	175.92 (19)	C10—N3—C14—C13	0.3 (5)
C2—C3—C4—O2	−178.1 (3)	Ag1—N3—C14—C13	161.4 (2)
C2—C3—C4—N1	2.4 (3)	C12—C13—C14—N3	−0.5 (5)
C9—N2—C5—C6	−0.2 (4)		

Fig. 1

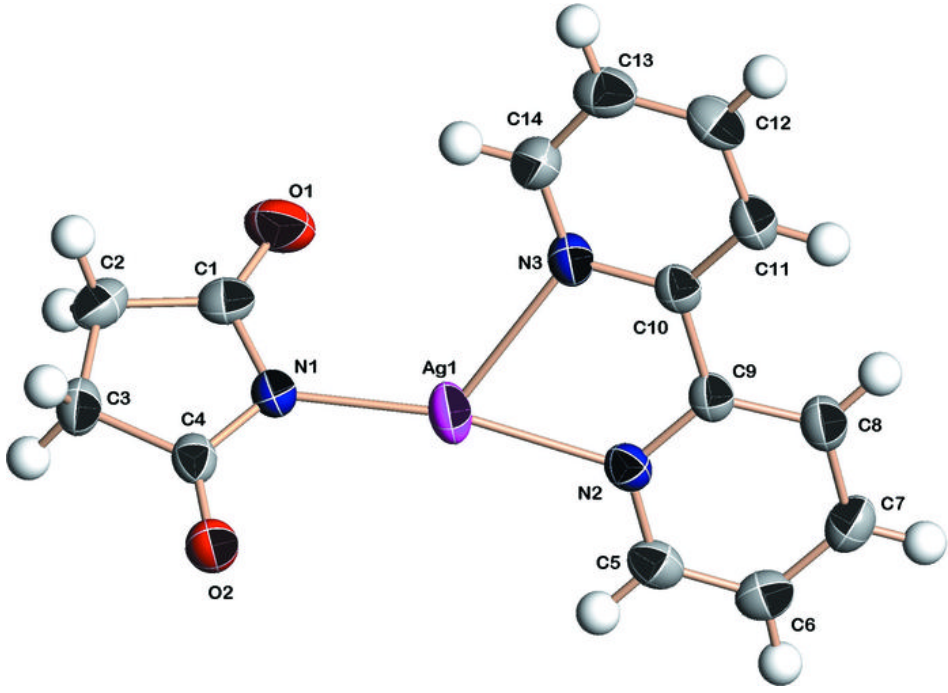


Fig. 2