Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(3-Aminopyridine-κN^1)(saccharinato-κN)silver(I)

Veysel T. Yilmaz,[a]* Sevim Hamamci[b] and Canan Kazak[c]

[a]Department of Chemistry, Faculty of Arts and Sciences, University of Uludag, 16059 Gorukle, Bursa, Turkey, [b]Department of Chemistry, Faculty of Arts and Sciences, Ondokuz Mayis University, 55019 Kurupelit, Samsun, Turkey, and [c]Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayis University, 55019 Kurupelit, Samsun, Turkey
Correspondence e-mail: vtyilmaz@uludag.edu.tr

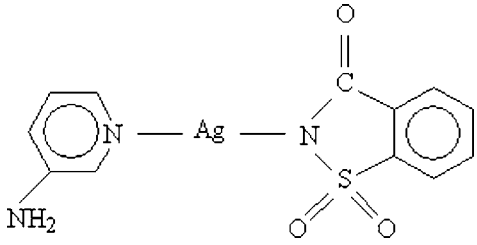
Received 7 November 2007; accepted 8 November 2007

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.023; wR factor = 0.061; data-to-parameter ratio = 16.9.

The Ag^I atom in the title complex, $[Ag(C_7H_4NO_3S)(C_5H_6N_2)]$, adopts an almost linear AgN_2 geometry with a saccharinate anion and a 3-aminopyridine ligand. Discrete molecules are linked by N—H···O hydrogen bonds into a three-dimensional network.

Related literature

For background, see: Jansen (1987); Weber *et al.* (1993); Yilmaz *et al.* (2004); Baran & Yilmaz (2006).



Experimental

Crystal data

$[Ag(C_7H_4NO_3S)(C_5H_6N_2)]$
M_r = 384.17
Triclinic, $P\overline{1}$
a = 6.7294 (7) Å
b = 8.0205 (8) Å
c = 13.5187 (14) Å
α = 82.149 (8)°
β = 80.111 (8)°
γ = 65.952 (7)°
V = 654.62 (12) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.71 mm^{-1}
T = 296 (2) K
0.52 × 0.45 × 0.33 mm

Data collection

Stoe IPDS2 diffractometer
Absorption correction: integration (*X-RED*; Stoe & Cie, 2002)
T_{min} = 0.466, T_{max} = 0.560
11027 measured reflections
3078 independent reflections
2773 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.061
S = 1.04
3078 reflections
182 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—N1	2.103 (2)	Ag1—N2	2.136 (2)
N1—Ag1—N2	170.00 (6)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···O3^{i}	0.86	2.48	3.251 (2)	149
N3—H3B···O1^{ii}	0.86	2.16	2.916 (2)	147

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

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2641).

References

Baran, E. J. & Yilmaz, V. T. (2006). *Coord. Chem. Rev.* **250**, 1980–1999.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Jansen, M. (1987). *Angew. Chem. Int. Ed. Engl.* **26**, 1098–1110.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Stoe & Cie (2002). *X-AREA* (Version 1.18) and *X-RED* (Version 1.04). Stoe & Cie, Darmstadt, Germany.
Weber, R., Gilles, M. & Bergerhoff, G. (1993). *Z. Kristallogr.* **206**, 273–274.
Yilmaz, V. T., Hamamci, S. & Thone, C. (2004). *Z. Anorg. Allg. Chem.* **630**, 1641–1644.

  doi:10.1107/S1600536807057248

supplementary materials

Acta Cryst. (2007). E**63**, m3000 [**doi:10.1107/S1600536807057248**]

(3-Aminopyridine-κN^1)(saccharinato-κN)silver(I)

V. T. Yilmaz, S. Hamamci and C. Kazak

Comment

Saccharin is a well known artificial sweetener and its deprotonated form, the saccharinate ion (sac), shows interesting ligation properties (Baran & Yilmaz 2006). Two different silver(I) complex of sac were reported by Weber *et al.* (1993) and Yilmaz *et al.* (2004). As part of our studies of mixed-ligand silver(I)-sac complexes with pyridine derivaties, the title compound (I) was prepared and characterized.

As shown in (Fig. 1), the Ag^I atom in (I) is coordinated by a sac ion and a neutral 3-aminopyridine ligand. The coordination geometry of the Ag^I atom is two-coordinate (linear) (Table 1). The shortest Ag···Ag distance between adjacent molecules in the crystal is 3.529 (2) Å which is considerably longer than the upper limit of 3.30 Å suggested for an argentophilic interaction in the silver(I) complexes (Jansen, 1987). Individual molecules are connected by N—H···O hydrogen bonds, involving the amine H atoms of 3-aminopyridine and the carbonyl and sulfonyl O atoms of the sac anion, thus forming a three-dimensional network (Table 2).

Experimental

Na(sac)·$2H_2O$ (0.24 g, 1 mmol) and 3-aminopyridine (0.09 g, 1 mmol) were added to a 20 ml solution of $AgNO_3$ (0.17 g, 1 mmol) dissolved in a mixture of water and acetonitryl (1:1, *v*/*v*). The solution was stirred for an hour at room temperature. Colourless prisms of (I) were obtained after 3 days by slow evoparation of the solution at room temperature.

Refinement

All hydrogen atoms were placed in idealized locations (C—H = 0.93 Å, N—H = 0.86 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(parent atom).

Figures

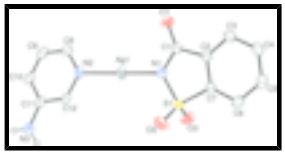


Fig. 1. The molecular structure of (I) showing 50% displacement ellipsoids (arbitrary spheres for the H atoms). The C-bound hydrogen atoms are omitted for clarity.

(3-Aminopyridine-κN^1)(saccharinato-KN)silver(I)

Crystal data

$[Ag(C_7H_4NO_3S)(C_5H_6N_2)]$ $Z = 2$

M_r = 384.17	F_{000} = 380
Triclinic, $P\bar{1}$	D_x = 1.949 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 6.7294 (7) Å	Cell parameters from 21946 reflections
b = 8.0205 (8) Å	θ = 2.8–28.0º
c = 13.5187 (14) Å	μ = 1.71 mm^{-1}
α = 82.149 (8)º	T = 296 (2) K
β = 80.111 (8)º	Prism, colourless
γ = 65.952 (7)º	0.52 × 0.45 × 0.33 mm
V = 654.62 (12) Å^3	

Data collection

Stoe IPDS 2 diffractometer	3078 independent reflections
Radiation source: fine-focus sealed tube	2773 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.044
Detector resolution: 6.67 pixels mm^{-1}	θ_{max} = 27.8º
T = 296(2) K	θ_{min} = 2.8º
rotation method scans	h = −8→8
Absorption correction: integration (X-RED; Stoe & Cie, 2002)	k = −10→10
T_{min} = 0.466, T_{max} = 0.560	l = −17→17
11027 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.023	$w = 1/[\sigma^2(F_o^2) + (0.0369P)^2 + 0.1071P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.061	$(\Delta/\sigma)_{max}$ = 0.014
S = 1.04	$\Delta\rho_{max}$ = 0.39 e Å^{-3}
3078 reflections	$\Delta\rho_{min}$ = −0.56 e Å^{-3}
182 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: 0.102 (3)
Secondary atom site location: difference Fourier map	

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}
C1	0.1263 (3)	1.0814 (3)	0.71084 (13)	0.0378 (4)
C2	0.0605 (3)	1.1547 (3)	0.81218 (13)	0.0370 (4)
C3	−0.1290 (3)	1.3000 (3)	0.84509 (16)	0.0478 (5)
H3	−0.2373	1.3625	0.8034	0.057*
C4	−0.1522 (4)	1.3493 (3)	0.94175 (18)	0.0571 (6)
H4	−0.2770	1.4476	0.9652	0.068*
C5	0.0064 (4)	1.2554 (4)	1.00394 (17)	0.0588 (6)
H5	−0.0143	1.2910	1.0688	0.071*
C6	0.1957 (4)	1.1095 (4)	0.97232 (16)	0.0511 (5)
H6	0.3024	1.0453	1.0145	0.061*
C7	0.2184 (3)	1.0637 (3)	0.87496 (14)	0.0389 (4)
C8	0.5785 (4)	0.6660 (3)	0.36057 (16)	0.0463 (4)
H8	0.4612	0.7748	0.3467	0.056*
C9	0.6889 (4)	0.5513 (3)	0.28488 (15)	0.0511 (5)
H9	0.6458	0.5825	0.2208	0.061*
C10	0.8629 (4)	0.3906 (3)	0.30389 (15)	0.0471 (4)
H10	0.9409	0.3138	0.2525	0.057*
C11	0.9213 (3)	0.3438 (3)	0.40059 (14)	0.0384 (4)
C12	0.8017 (3)	0.4666 (3)	0.47316 (13)	0.0371 (4)
H12	0.8390	0.4372	0.5383	0.044*
N1	0.3306 (3)	0.9470 (2)	0.70220 (12)	0.0415 (3)
N2	0.6354 (3)	0.6253 (2)	0.45379 (12)	0.0400 (3)
N3	1.0955 (3)	0.1840 (3)	0.42523 (14)	0.0503 (4)
H3A	1.1720	0.1096	0.3798	0.060*
H3B	1.1271	0.1593	0.4860	0.060*
O1	0.0082 (3)	1.1362 (2)	0.64384 (11)	0.0520 (4)
O2	0.4685 (3)	0.7160 (2)	0.84633 (14)	0.0675 (5)
O3	0.6308 (3)	0.9409 (3)	0.79346 (13)	0.0614 (4)
S1	0.43996 (8)	0.89815 (7)	0.80659 (4)	0.04355 (12)
Ag1	0.49733 (3)	0.80193 (2)	0.574282 (11)	0.04861 (9)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0397 (9)	0.0380 (9)	0.0337 (8)	−0.0128 (7)	−0.0045 (7)	−0.0046 (7)
C2	0.0367 (9)	0.0388 (9)	0.0327 (8)	−0.0116 (7)	−0.0037 (7)	−0.0046 (7)
C3	0.0398 (10)	0.0461 (10)	0.0460 (10)	−0.0054 (8)	−0.0040 (8)	−0.0053 (8)
C4	0.0512 (12)	0.0544 (12)	0.0496 (12)	−0.0054 (10)	0.0067 (9)	−0.0174 (10)
C5	0.0631 (14)	0.0688 (15)	0.0387 (10)	−0.0190 (12)	0.0039 (9)	−0.0203 (10)

C6	0.0467 (11)	0.0682 (14)	0.0348 (9)	−0.0166 (10)	−0.0067 (8)	−0.0090 (9)
C7	0.0349 (9)	0.0432 (9)	0.0340 (8)	−0.0102 (7)	−0.0027 (7)	−0.0069 (7)
C8	0.0473 (11)	0.0473 (11)	0.0455 (10)	−0.0196 (9)	−0.0075 (8)	−0.0023 (8)
C9	0.0610 (13)	0.0641 (13)	0.0342 (9)	−0.0291 (11)	−0.0089 (9)	−0.0049 (9)
C10	0.0529 (11)	0.0581 (12)	0.0340 (9)	−0.0238 (10)	−0.0014 (8)	−0.0142 (8)
C11	0.0376 (9)	0.0460 (10)	0.0364 (8)	−0.0207 (8)	0.0006 (7)	−0.0121 (7)
C12	0.0374 (9)	0.0456 (10)	0.0330 (8)	−0.0205 (8)	−0.0007 (7)	−0.0101 (7)
N1	0.0412 (8)	0.0436 (8)	0.0340 (7)	−0.0090 (7)	−0.0035 (6)	−0.0110 (6)
N2	0.0385 (8)	0.0453 (8)	0.0389 (8)	−0.0191 (7)	0.0015 (6)	−0.0114 (7)
N3	0.0451 (9)	0.0541 (10)	0.0453 (9)	−0.0084 (8)	−0.0050 (7)	−0.0192 (8)
O1	0.0499 (8)	0.0629 (9)	0.0390 (7)	−0.0139 (7)	−0.0143 (6)	−0.0060 (6)
O2	0.0731 (11)	0.0435 (8)	0.0581 (10)	0.0030 (8)	−0.0080 (8)	0.0024 (7)
O3	0.0366 (7)	0.0903 (13)	0.0507 (8)	−0.0148 (8)	−0.0054 (6)	−0.0166 (8)
S1	0.0372 (2)	0.0457 (3)	0.0351 (2)	−0.00214 (19)	−0.00529 (17)	−0.00619 (18)
Ag1	0.05145 (12)	0.04605 (11)	0.04045 (11)	−0.01003 (7)	0.00057 (6)	−0.01523 (6)

Geometric parameters (Å, °)

C1—O1	1.224 (2)	C8—H8	0.9300
C1—N1	1.355 (2)	C9—C10	1.371 (3)
C1—C2	1.489 (2)	C9—H9	0.9300
C2—C7	1.375 (3)	C10—C11	1.388 (3)
C2—C3	1.385 (3)	C10—H10	0.9300
C3—C4	1.382 (3)	C11—N3	1.386 (3)
C3—H3	0.9300	C11—C12	1.388 (2)
C4—C5	1.376 (4)	C12—N2	1.338 (3)
C4—H4	0.9300	C12—H12	0.9300
C5—C6	1.382 (3)	N1—S1	1.6301 (17)
C5—H5	0.9300	N3—H3A	0.8600
C6—C7	1.381 (3)	N3—H3B	0.8600
C6—H6	0.9300	O2—S1	1.4322 (19)
C7—S1	1.7576 (19)	O3—S1	1.4361 (18)
C8—N2	1.339 (3)	Ag1—N1	2.103 (2)
C8—C9	1.373 (3)	Ag1—N2	2.136 (2)
O1—C1—N1	124.38 (18)	C8—C9—H9	120.0
O1—C1—C2	123.60 (17)	C9—C10—C11	119.28 (19)
N1—C1—C2	112.02 (15)	C9—C10—H10	120.4
C7—C2—C3	120.21 (17)	C11—C10—H10	120.4
C7—C2—C1	112.00 (15)	N3—C11—C10	122.46 (18)
C3—C2—C1	127.75 (17)	N3—C11—C12	120.05 (18)
C4—C3—C2	117.9 (2)	C10—C11—C12	117.46 (19)
C4—C3—H3	121.1	N2—C12—C11	123.09 (17)
C2—C3—H3	121.1	N2—C12—H12	118.5
C5—C4—C3	121.1 (2)	C11—C12—H12	118.5
C5—C4—H4	119.4	C1—N1—S1	112.45 (13)
C3—C4—H4	119.4	C1—N1—Ag1	126.52 (13)
C4—C5—C6	121.6 (2)	S1—N1—Ag1	120.98 (9)
C4—C5—H5	119.2	C12—N2—C8	118.52 (17)
C6—C5—H5	119.2	C12—N2—Ag1	115.95 (12)

C7—C6—C5	116.7 (2)	C8—N2—Ag1	125.39 (15)
C7—C6—H6	121.7	C11—N3—H3A	120.0
C5—C6—H6	121.7	C11—N3—H3B	120.0
C2—C7—C6	122.51 (18)	H3A—N3—H3B	120.0
C2—C7—S1	107.76 (13)	O2—S1—O3	116.39 (12)
C6—C7—S1	129.68 (16)	O2—S1—N1	110.23 (11)
N2—C8—C9	121.7 (2)	O3—S1—N1	110.56 (10)
N2—C8—H8	119.1	O2—S1—C7	111.72 (10)
C9—C8—H8	119.1	O3—S1—C7	110.33 (10)
C10—C9—C8	119.90 (19)	N1—S1—C7	95.70 (9)
C10—C9—H9	120.0	N1—Ag1—N2	170.00 (6)
O1—C1—C2—C7	177.0 (2)	O1—C1—N1—Ag1	0.7 (3)
N1—C1—C2—C7	−2.7 (2)	C2—C1—N1—Ag1	−179.66 (13)
O1—C1—C2—C3	−5.2 (3)	C11—C12—N2—C8	1.4 (3)
N1—C1—C2—C3	175.2 (2)	C11—C12—N2—Ag1	−174.39 (14)
C7—C2—C3—C4	0.2 (3)	C9—C8—N2—C12	−1.3 (3)
C1—C2—C3—C4	−177.5 (2)	C9—C8—N2—Ag1	174.05 (16)
C2—C3—C4—C5	−0.9 (4)	C1—N1—S1—O2	113.94 (16)
C3—C4—C5—C6	0.6 (4)	Ag1—N1—S1—O2	−63.80 (14)
C4—C5—C6—C7	0.5 (4)	C1—N1—S1—O3	−115.95 (16)
C3—C2—C7—C6	0.9 (3)	Ag1—N1—S1—O3	66.30 (14)
C1—C2—C7—C6	178.9 (2)	C1—N1—S1—C7	−1.73 (16)
C3—C2—C7—S1	−176.67 (17)	Ag1—N1—S1—C7	−179.47 (11)
C1—C2—C7—S1	1.3 (2)	C2—C7—S1—O2	−114.31 (16)
C5—C6—C7—C2	−1.3 (3)	C6—C7—S1—O2	68.3 (2)
C5—C6—C7—S1	175.75 (19)	C2—C7—S1—O3	114.56 (15)
N2—C8—C9—C10	−0.3 (3)	C6—C7—S1—O3	−62.8 (2)
C8—C9—C10—C11	1.8 (3)	C2—C7—S1—N1	0.14 (16)
C9—C10—C11—N3	−179.8 (2)	C6—C7—S1—N1	−177.2 (2)
C9—C10—C11—C12	−1.6 (3)	C1—N1—Ag1—N2	−83.7 (4)
N3—C11—C12—N2	178.24 (18)	S1—N1—Ag1—N2	93.8 (4)
C10—C11—C12—N2	0.1 (3)	C12—N2—Ag1—N1	−81.7 (4)
O1—C1—N1—S1	−176.92 (18)	C8—N2—Ag1—N1	102.8 (4)
C2—C1—N1—S1	2.7 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3A···O3^{i}	0.86	2.48	3.251 (2)	149
N3—H3B···O1^{ii}	0.86	2.16	2.916 (2)	147

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

Fig. 1