New Triazoloquinoxaline Ligand and its Polymeric 1D Silver(I) complex

Synthesis, Structure, and Antimicrobial activity

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Supplementary informations

Table S1. Crystal data and structure refinement for compounds **1** and **2**.

	L (1)	**$[Ag_2L(NO_3)_2]_n$ (2)**
Empirical formula	$C_{18}H_{17}N_5$	$C_{18}H_{17}N_7Ag_2O_6$
Formula weight	303.37	643.13
Temperature	298(2) K	298(2) K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Triclinic	Monoclinic
Space group	P1	$P2_1/n$
Unit cell dimensions	a = 11.496(2) Å b = 12.436(3) Å c = 13.615(3) Å α = 94.96(3)° β = 110.83(3)° γ = 116.22(3)°	a = 14.932(3) Å b = 10.070(2) Å c = 15.112(3) Å α = 90° β =113.25(3)° γ = 90°
Volume	1561.6(10) $Å^3$	2087.8(9) $Å^3$
Z	4	4
Density (calculated)	1.290 Mg/m^3	2.046 Mg/m^3
Absorption coefficient	0.081 mm^{-1}	1.929 mm^{-1}
F(000)	640	1264
Theta range for data collection	3.09 to 22.45°	2.93 to 25.00°
Index ranges	-11<=h<=12 -13<=k<=13 -14<=l<=14	-17<=h<=17 -10<=k<=10 -17<=l<=17
Reflections collected	6891	5413
Independent reflections	4030 [R(int) = 0.0547]	3369 [R(int) = 0.0661]
Completeness up to theta =	22.45°, 98.8 %	25.00°, 92.0 %
Absorption correction	Semi-empirical from equivalents	

Refinement method	Full-matrix least-squares on F2	
Data / restraints / parameters	4030 / 0 / 420	3369 / 0 / 295
Goodness-of-fit on F^2	1.007	1.012
Final R indices [I>2σ(I)]	R1 = 0.0515, wR2 = 0.1009	R1 = 0.0658, wR2 = 0.1585
R indices (all data)	R1 = 0.1170, wR2 = 0.1257	R1 = 0.1007, wR2 = 0.1819
Extinction coefficient	0.0078(12)	---
Largest diff. peak and hole	0.154 and -0.144 e.Å^{-3}	1.267 and -1.207 e.Å^{-3}

Table S2 Selected bond lengths [Å] and angles [°] for **(1)**. The values for only one molecule (A) in the asymmetric unit are given; the parameters of the second molecular unit are comparable.

C(1)-N(1)	1.315(4)	C(4)-C(5)	1.397(4)	C(12)-C(13)	1.518(5)
C(1)-N(3)	1.382(4)	C(4)-N(4)	1.402(4)	C(13)-C(14)	1.379(5)
C(1)-N(5)	1.385(4)	C(5)-C(6)	1.387(4)	C(13)-C(18)	1.381(5)
C(2)-N(2)	1.321(4)	C(5)-N(3)	1.403(4)	C(14)-C(15)	1.385(5)
C(2)-N(3)	1.376(4)	C(6)-C(7)	1.367(4)	C(15)-C(16)	1.361(5)
C(2)-C(3)	1.430(5)	C(7)-C(8)	1.373(5)	C(16)-C(17)	1.366(5)
C(3)-N(4)	1.294(4)	C(8)-C(9)	1.368(5)	C(16)-C(17)	1.366(5)
C(3)-C(12)	1.511(4)	C(10)-N(5)	1.465(4)	C(17)-C(18)	1.377(5)
C(4)-C(9)	1.395(5)	C(11)-N(5)	1.466(4)	N(1)-N(2)	1.398(4)
N(1)-C(1)-N(3)	110.4(3)	C(4)-C(5)-N(3)	115.3(3)		
N(1)-C(1)-N(5)	127.5(3)	C(7)-C(6)-C(5)	119.1(4)		
N(3)-C(1)-N(5)	122.1(3)	C(6)-C(7)-C(8)	120.5(4)		
N(2)-C(2)-N(3)	110.8(3)	C(9)-C(8)-C(7)	120.7(4)		
N(2)-C(2)-C(3)	129.7(3)	C(8)-C(9)-C(4)	120.5(4)		
N(3)-C(2)-C(3)	119.4(3)	C(3)-C(12)-C(13)	109.0(3)		
N(4)-C(3)-C(2)	121.4(3)	C(14)-C(13)-C(18)	117.7(4)		

N(4)-C(3)-C(12)	119.9(3)	C(14)-C(13)-C(12)	121.8(4)
C(2)-C(3)-C(12)	118.6(3)	C(18)-C(13)-C(12)	120.4(3)
C(9)-C(4)-C(5)	117.7(3)	C(13)-C(14)-C(15)	120.6(4)
C(9)-C(4)-N(4)	118.3(4)	C(16)-C(15)-C(14)	121.0(4)
C(5)-C(4)-N(4)	124.0(3)	C(15)-C(16)-C(17)	118.9(4)
C(6)-C(5)-C(4)	121.3(3)	C(16)-C(17)-C(18)	120.6(4)
C(6)-C(5)-N(3)	123.4(3)	C(17)-C(18)-C(13)	121.2(3)

Table S3 Selected bond lengths [Å] and angles [°] for **(2)**. Only bond angles involving silver atoms and those of the nitrate ions are listed.

Ag(1)-N(2)#1	2.243(6)	Ag(2)-N(1)	2.239(6)
Ag(1)-N(4)	2.264(6)	Ag(2)-O(4)	2.338(8)
Ag(1)-O(1)	2.369(7)	Ag(2)-O(1)#2	2.389(7)
Ag(1)-C(13)	2.717(8)	Ag(2)-O(5)	2.610(7)
Ag(1)-C(14)	2.897(9)	Ag(2)-O2A	2.82(2)
Ag(1)-C(18)	3.002(9)	Ag(2)-C(16)	3.085(9)

N(1)-N(2)	1.396(8)	N(3)-C(5)	1.420(9)	C(6)-C(7)	1.378(13)
N(2)-C(2)	1.301(9)	N(4)-C(3)	1.302(9)	C(7)-C(8)	1.376(13)
N(3)-C(2)	1.355(9)	C(4)-C(5)	1.385(11)	C(8)-C(9)	1.370(13)
N(3)-C(1)	1.401(9)	C(5)-C(6)	1.396(12)	C(12)-C(13)	1.527(10)
O(1)-N(6)	1.276(10)	N(4)-C(4)	1.416(10)	C(13)-C(18)	1.374(11)
O(2A)-N(6)	1.262(18)	N(5)-C(1)	1.373(10)	C(13)-C(14)	1.380(12)
O(3A)-N(6)	1.260(20)	N(5)-C(11)	1.445(11)	C(14)-C(15)	1.392(13)
O(4)-N(7)	1.258(9)	N(5)-C(10)	1.459(11)	C(15)-C(16)	1.343(15)
O(5)-N(7)	1.223(10)	C(2)-C(3)	1.444(10)	C(16)-C(17)	1.378(14)
O(6)-N(7)	1.218(9)	C(3)-C(12)	1.475(11)	C(17)-C(18)	1.368(12)
N(1)-C(1)	1.311(10)	C(4)-C(9)	1.367(11)	N(1)-C(1)	1.311(10)

N(2)#1-Ag(1)-N(4)	138.7(2)	N(2)-N(1)-Ag(2)	117.0(5)
N(2)#1-Ag(1)-O(1)	93.5(3)	C(2)-N(2)-Ag(1)#2	134.6(5)
N(4)-Ag(1)-O(1)	122.9(2)	N(1)-N(2)-Ag(1)#2	118.0(5)
N(1)-Ag(2)-O(4)	134.4(2)	C(3)-N(4)-Ag(1)	120.7(5)
N(1)-Ag(2)-O(1)#2	96.0(2)	C(4)-N(4)-Ag(1)	115.6(5)
O(4)-Ag(2)-O(1)#2	126.4(3)	O(2A)-N(6)-O(3A)	124.0(12)
N(6)-O(1)-Ag(1)	133.7(6)	O(2A)-N(6)-O(1)	109.1(11)
N(6)-O(1)-Ag(2)#1	113.4(5)	O(3A)-N(6)-O(1)	126.9(11)
Ag(1)-O(1)-Ag(2)#1	94.8(2)	O(6)-N(7)-O(5)	121.7(9)
N(7)-O(4)-Ag(2)	103.1(6)	O(6)-N(7)-O(4)	122.2(8)
C(1)-N(1)-Ag(2)	131.0(5)	O(5)-N(7)-O(4)	116.1(8)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1/2,y+1/2,-z+3/2 #2 -x+1/2,y-1/2,-z+3/2