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Journal of Molecular Structure 733 (2005) 95–99

Journal of
MOLECULAR
STRUCTURE

www.elsevier.com/locate/molstruc

New silver(I) complexes of Schiff base with hydrogen-bonding interactions: effects of anions on the framework formations of complexes

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Received 10 June 2004; revised 11 August 2004; accepted 11 August 2004
Available online 25 September 2004

Abstract

Two new one-dimensional $\mathrm{Ag^I}$ complexes, $[\mathrm{Ag}\mathbf{L}(\mathrm{NO_3})]_\infty$ (**1**) and $\{[\mathrm{Ag}\mathbf{L}](\mathrm{ClO_4})\}_\infty$ (**2**) (**L**=*N*,*N*′-bis(2-hydroxyethy)-*p*-phenylenedimethyleneamine), have been synthesized and their structures were determined by single-crystal X-ray diffraction analysis. **1** crystallizes in the monoclinic system, space group *Cc*, with $a=13.305(5)$, $b=14.107(5)$, $c=7.608(3)$ Å, $\beta=97.226(6)°$ and $Z=4$, while **2** crystallizes in the monoclinic space group *C2/c*, with $a=12.902(5)$, $b=8.671(3)$, $c=27.776(11)$ Å, $\beta=97.796(6)°$ and $Z=8$. In **1**, the $\mathrm{Ag^I}$ atom adopts distorted $\mathrm{N_2O_2}$ tetrahedral coordination geometry, while in **2**, the $\mathrm{Ag^I}$ center is coordinated by two nitrogen atoms from two different **L** ligands. The structural differences of **1** and **2** suggest that counter anions have a profound effect upon the framework formations of $\mathrm{Ag^I}$ complexes with the ligand **L**. The strong and weak hydrogen-bonding interactions in **1** and **2** extend two one-dimensional complexes into two quasi two-dimensional networks, and such weak interactions further stabilized two complexes.

Keywords: Self-assembly; Schiff base; Silver(I) complexes; Crystal structure; Hydrogen bonds

1. Introduction

The self-assembly of metal ions with multi-topic ligands continues to be a theme of considerable current interest in the context of developing new solid-state polymeric materials with specific architectures and functions [1,2]. The self-assembly process of metal complexes is quite complicated and understanding the factors that affect the process between labile metal ions and flexible multidentate ligands is an interesting and challenging topic in supramolecular and coordination chemistry. Flexible multidentate bridging ligands have shown interesting coordination chemistry with transition metal ions [3]. Due to the flexibility of such ligands, they are very sensitive to the changes of conditions employed and may result in different coordination modes and complexes with different architectures [4–6].

Metal complexes of Schiff bases have been playing an important part in the development of coordination chemistry as a whole since the first synthesis of Schiff base metal complexes was reported by Professor H. Schiff in 1869 [7]. The metal complexes of Schiff bases have been of interest for many years due to their homogeneous catalysis and enzymatic reactions, antibacterial activities, magnetism and molecular architectures [8–11]. In this paper, we synthesized a new Schiff base ligand **L** (**L**=*N*,*N*′-bis(2-hydroxyethy)-*p*-phenylenedimethyleneamine). Herein, we report two $\mathrm{Ag^I}$ coordination architectures with the ligand, and the effects of anions on the structures of complexes have also been discussed.

2. Experimental

2.1. Materials and general methods

All reagents for syntheses and analyses were of analytical grade. FT-IR spectra (KBr pellet) were obtained on a FT-IR 170 SX (Nicolet) spectrometer. Elemental analyses were

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doi:10.1016/j.molstruc.2004.08.007

taken using a Perkin–Elmer 240C analyzer. ^{1}H NMR spectra were recorded on a Bruker AC-P500 spectrometer (300 MHz) at 25 °C in $CDCl_3$ with tetramethylsilane as the internal reference.

Caution. Although no problems were encountered in the preparation of the perchlorate salt, care should be taken when handing such a potentially explosive compound.

2.2. Syntheses of the ligand **L**

To a solution of isophthalaldehyde (1.68 g, 12.5 mmol) in dried MeOH (20 ml) was added a solution of ethanolamine (1.53 g, 25 mmol) in dried MeOH (5 ml). The mixture was stirred for 3 h at room temperature, and a white precipitate was obtained. The solid product was washed with MeOH and dried in vacuum to obtain ligand **L** with a yield of 60%. m.p. 141–142 °C. Anal. Calc. for $C_{12}H_{16}N_2O_2$: C 65.43, H 7.32, N 12.72; Found: C 65.47, H 7.29, N 12.76. FT-IR (KBr, cm^{-1}): 3192w, 1647s, 1559m, 1540m, 1507ms, 1458mm, 1068s, 871m, 832m, 713m. ^{1}H NMR (300 MHz, $CDCl_3$): δ8.38 (2H, CH=N), 7.79–7.26 (4H, arom), 5.46 (1H, OH), 3.96–3.88 (4H, OCH_2), 3.82–3.78 (4H, $=NCH_2$) Scheme 1.

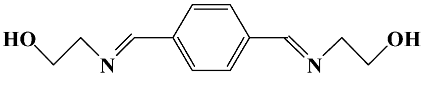
2.3. Preparation of $[Ag\mathbf{L}(NO_3)]_\infty$ (**1**) and $[Ag\mathbf{L}(ClO_4)]_\infty$ (**2**)

2.3.1. $[AgL(NO_3)]_\infty$ (**1**)

A solution of $AgNO_3$ (17 mg, 0.1 mmol) in MeCN (2 ml) was added to a stirred solution of **L** (22 mg, 0.1 mmol) in MeOH (6 ml) and CH_2Cl_2 (2 ml). The mixture was refluxed at 50 °C for 3 h to give a clear mixture. Slow diffusion of diethyl ether into the resulting solution for 3 days produced colorless crystal with 32% yield. Anal. Calc. for $C_{12}H_{16}AgN_3O_5$: C 36.94, H 4.13, N 10.77; Found: C 36.80, H 4.07, N 10.95. FT-IR (KBr, cm^{-1}): 3442s, 1659s, 1613s, 1454, 1384s, 1121m, 1068, 831m, 668m.

2.3.2. $\{[AgL](ClO_4)\}_\infty$ (**2**)

The analogous reaction of $AgClO_3$ with **L** produced colorless block crystals of **2** with 48% yield. Anal. Calc. for $C_{12}H_{16}AgClN_2O_6$: C 33.71, H 3.77, N 6.55; Found: C 33.65, H 3.88 N 6.39. FT-IR (KBr, cm^{-1}): 3650m, 3196m, 2909m, 1646s, 1570m, 1560m, 1508m, 1498m, 1458m, 1113s, 870m, 831m, 669.



L

Scheme 1. The structural diagram of the **L** ligand.

Table 1
Crystal data and structure refinement summary for **1** and **2**

Empirical formula	C1$_{12}$H$_{16}$AgN$_3$O$_5$	$C_{12}H_{16}AgClN_2O$
Formula weight	390.15	427.59
Crystal system	Monoclinic	Monoclinic
Space group	*Cc*	*C2/c*
Unit cell dimensions (Å, degrees)	$a=13.305(5)$ $b=14.107(5)$ $c=7.608(3)$ $\beta=97.226(6)$	$a=12.902(5)$ $b=8.671(3)$ $c=27.776(11)$ $\beta=97.796(6)$
Volume (Å^3)	1416.6(8)	3079(2)
Z	4	8
D_{calc} (g/cm^3)	1.829	1.845
μ (mm^{-1})	1.448	1.512
F(000)	784	1712
Range of h, k, l	$-16/15$, $-17/17$, $-9/7$	$-12/15$, $-9/10$, $-29/33$
Reflections collected/ unique	3987/1850	7675/2709
Max. and min. transmission	1.0000 and 0.7998	1.0000 and 0.8433
Data/restraints/ parameters	1850/2/191	2709/24/211
Goodness-of-fit on F^2	1.047	1.142
R and R_w	0.0231 and 0.0482	0.0499 and 0.1348
Largest diff. Peak and hole (e/Å^3)	0.494 and -0.267	0.888 and -0.619

2.4. X-ray crystallographic study of metal complexes

Diffraction intensities for complexes **1** and **2** were collected on a Bruker Smart 1000 CCD area detector using graphite-monochromatized Mo Kα radiation ($\lambda=0.71073$ Å) with ω scan mode at 293(2) K. Unit cell dimensions were obtained with least-squares refinements and semi-empirical absorption corrections were applied using SADABS program [12]. All the structures were solved by direct method [13] and non-hydrogen atoms were obtained in successive difference Fourier syntheses. The final refinements were performed by full-matrix least-squares methods on F^2 by SHELXL-97 program package [14]. Hydrogen atoms were included in calculated positions and refined with fixed thermal parameters riding on their parent atoms. Further crystallographic data and experimental details for structural analyses are summarized in Table 1, and positional parameters and atomic coordinates are given in Table 2. CCDC-236453 and CCDC-236454 contain the supplementary crystallographic data for complexes **1** and **2**, respectively. These data can be obtained from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; Fax: +44-1223-336033; E-mail: deposit@ccdc.cam.ac.uk.

3. Results and discussion

3.1. Syntheses and general methods

Complexes **1** and **2** were synthesized by self-assembly of AgX ($X=NO_3^-$, ClO_4^-) salts with **L** ligand. The IR spectra of the two complexes show that the absorption bands resulting from the skeletal vibrations of aromatic