

Coordination complexes built with 3-nitrophthalate and different pyrazine derivatives: Syntheses, structures and photoluminescence



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ARTICLE INFO

Article history:

Received 3 November 2014

Received in revised form 4 January 2015

Accepted 9 January 2015

Available online 19 January 2015

Keywords:

Silver(I) complexes
Pyrazine derivatives
Coordination complex
Photoluminescence

ABSTRACT

Three Ag(I) coordination complexes (CCs), namely $\{Ag_2(epy_z)(npt)\}_n$ (**1**), $\{Ag_2(tpyz)(npt)\}_n$ (**2**), $\{Ag_2(npt)(NH_3)_2\}_n$ (**3**), [epy_z = 2-ethyl-3-methylpyrazine, H_2npt = 3-nitro-1,2-benzenedicarboxylic acid, $tpyz$ = 2,3,5-trimethylpyrazine, $mpyz$ = 2,3,5,6-tetramethylpyrazine] have been synthesized by solution phase ultrasonic reactions of Ag_2O with H_2npt and various pyrazine derivatives ligands under the ammoniacal condition. All the complexes have been characterized by X-ray diffraction, elemental analyses and IR spectra. Complexes **1** and **2** show two-dimensional network. Compound **3** exhibits 1D-chain structure. However, complex **3** shows 3D supramolecular structure results from the linkage of neighboring layers through a rich hydrogen-bonding system involving the ammonia molecules with carboxyl oxygen atoms and the nitro oxygen atoms. Zigzag Ag_4 subunits (SBUs) were observed in compounds **1** and **3**, while the complex **2** only shows $Ag_2 \cdots Ag_2$ interactions. The structural diversity of the compounds indicated the $Ag \cdots Ag$ argentophilicity, the coordination modes of carboxyl groups and the difference pyrazine derivatives play an important role in the formation of such coordination architectures. The thermogravimetric analyses and photoluminescence of the complexes were also investigated.

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1. Introduction

The design and synthesis of Ag(I) coordination complexes [1–7] have attracted great attention in the recently years because of the versatility of their coordination geometries [8]. Meanwhile, the design and construction of mixed-ligand coordination polymers [9–12] are also considerable interest in the recent years due to their potential use in adsorption, host–guest chemistry, catalysis, and electrofunctional materials [13–17]. It seems interesting to change the kinds of the N-containing ligands and dicarboxylates because of their ability to create unusual structures with important properties [18–21]. On the basis of our previous reports, carboxyl groups can be partially or completely deprotonated and can coordinate with Ag(I) in different coordination modes, such as monodentate, chelating and bridging [22–25]. On the other hand, pyrazine derivatives are divergent bidentate ligands and commonly act as bridging ligands. Some silver coordination polymers containing pyrazine derivatives ligands with different topologies have been reported [26–29].

In this paper, we chose H_2npt as auxiliary ligand in the construction of coordination complexes because of its special features.

And three pyrazine derivatives were selected as neutral ligands to construct novel silver coordination complexes and study their effects on the structures of compounds. Three compounds, namely, $\{Ag_2(epy_z)(npt)\}_n$ (**1**), $\{Ag_2(tpyz)(npt)\}_n$ (**2**), $\{Ag_2(npt)(NH_3)_2\}_n$ (**3**) have been synthesized. The preparation routes of three coordination compounds which is represented in Scheme 1. The crystal structures of these compounds have been determined by single-crystal X-ray diffraction and characterized by IR and elemental analyses. The thermogravimetric analyses and luminescent properties of these compounds were also studied.

2. Experimental

2.1. Materials and physical measurements

All solvents and reagents which were employed in the syntheses were of analytical grade and they were used without further purification. Elemental analyses for C, H, N were measured on a CE instruments EA 1110 elemental analyzer. IR spectra were carried out on a Nicolet Avatar 330 FTIR Spectrometer as KBr pellets in the frequency range of $4000\text{--}400\text{ cm}^{-1}$. Photoluminescent properties were measured on a Hitachi F-7000 Fluorescence Spectrophotometer with solid powder on a 1 cm quartz round

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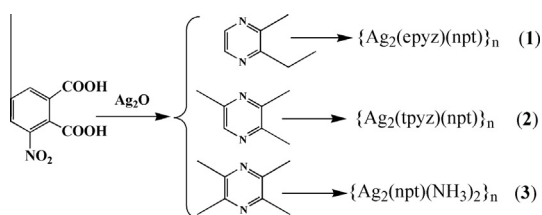
plate. X-ray powder diffractions were measured on a Panalytical X-Pert pro diffractometer with Cu K α radiation. TG curves were measured from 25 to 800 °C on a SDT Q600 instrument at a heating rate of 10 °C min⁻¹ under N₂ atmosphere (100 mL min⁻¹).

2.2. Synthesis of complex {Ag₂(epyz)(npt)}_n (**1**)

Ag₂O (23.2 mg, 0.1 mmol), 3-nitro-1,2-benzenedicarboxylic acid (H₂npt) (42.2 mg, 0.2 mmol) and epyz (24.4 mg, 0.2 mmol) were dissolved in methanol-H₂O-DMF mixed solvent (6 mL, v/v/v = 1/1/1) in the presence of ammonia (0.5 mL, 14 M) under ultrasonic treatment (160 W, 40 kHz, 30 min) under 40 °C. The resultant colorless solution was allowed slowly to evaporate at room temperature in the dark. After several days, colorless plate crystals of **1** were isolated in about a 43% yield. They were washed with a small volume of cold ethanol. *Anal.* Calc. for Ag₂C₁₅H₁₃N₃O₆: C, 32.94; H, 2.40; N, 7.68. Found: C, 32.98; H, 2.38; N, 7.72%. IR (KBr): ν (cm⁻¹) = 3440 (m), 3088 (w), 3046 (w), 2976 (m), 2932 (w), 2876 (w), 1590 (s), 1520 (s), 1457 (s), 1408 (s), 1344 (s), 1288 (m), 1162 (m), 1027 (w), 929 (m), 859 (m), 824 (m), 782 (w), 747 (w), 704 (m), 683 (m), 586 (w).

2.3. Synthesis of complex {Ag₂(tpyz)(npt)}_n (**2**)

The synthesis of **2** was similar to that of **1**, but with tpyz (24.4 mg, 0.2 mmol) in place of epyz in the same mixed solvent. Colorless plate crystals of **2** were obtained in 62% yield. *Anal.* Calc. for Ag₂C₁₅H₁₃N₃O₆: C, 32.94; H, 2.40; N, 7.68. Found: C, 32.83; H,



Scheme 1. The preparation routes of three coordination compounds **1–3**.

2.44; N, 7.84%. IR (KBr): ν (cm⁻¹) = 3432 (m), 3067 (m), 2926 (w), 1590 (s), 1526 (s), 1449 (s), 1352 (s), 1294 (w), 1176 (m), 1070 (w), 1006 (w), 929 (m), 824 (m), 788 (w), 760 (m), 718 (s), 683 (m), 592 (w), 444 (w).

2.4. Synthesis of complex {Ag₂(npt)(NH₃)₂}_n (**3**)

The synthesis of **3** was similar to that of **1**, but with mpyz (27.2 mg, 0.2 mmol) in place of epyz and the mixed solvent is DMF-methanol. Colorless prism crystals of **3** were obtained in 47% yield. *Anal.* Calc. for Ag₂C₈H₉N₃O₆: C, 20.92; H, 1.96; N, 9.15. Found: C, 20.83; H, 1.72; N, 9.11%. IR (KBr): ν (cm⁻¹) = 3326 (m), 1604 (s), 1534 (s), 1457 (m), 1387 (s), 1344 (s), 1294 (w), 1217 (w), 1155 (w), 929 (w), 824 (m), 788 (w), 753 (w), 712 (m), 683 (w), 585 (w), 430 (w).

2.5. X-ray crystallography

Crystallographic data of compounds **1–3** were collected on Rigaku R-Axis RAPID imaging Plate single-crystal diffractometer with graphite-monochromated Mo K α radiation source (λ = 0.71073 Å) operating at 50 kV and 90 mA in ω scan mode. The crystal structures were solved and refined using Fullmatrix least-squares based on F₂ with program SHELXS-97 [30] and SHELXL-97 [31] within OLEX2 [32]. Absorption correction was applied by correction of symmetry-equivalent reflections using the ABCOR program [33]. In all cases, the highest possible space group was chosen.

Atoms were located from iterative examination of difference F-maps following least squares refinements of the earlier models. Hydrogen atoms were placed in calculated positions and included as riding atoms with isotropic displacement parameters 1.2–1.5 times U_{eq} of the attached C or N atoms. The hydrogen atoms attached to oxygen were refined with O–H = 0.85 Å, and U_{iso}(H) = 1.2 U_{eq}(O). All structures were examined using the Addsym subroutine of PLATON [34] to assure that no additional symmetry could be applied to the models. Pertinent crystallographic data collections and refinement parameters are collated in Table 1. Selected bond lengths and angles for **1–3** are collated in Table 2.

Table 1
Crystallographic data for complexes **1–3**.

Complexes	1	2	3
Formula	Ag ₂ C ₁₅ H ₁₃ N ₃ O ₆	Ag ₂ C ₁₅ H ₁₃ N ₃ O ₆	Ag ₂ C ₈ H ₉ N ₃ O ₆
<i>M_r</i>	547.02	547.02	458.92
Crystal system	triclinic	orthorhombic	monoclinic
Space group	<i>P</i> $\bar{1}$	<i>Pbna</i>	<i>P2₁/n</i>
<i>a</i> (Å)	7.3027(10)	9.6840(10)	7.169(2)
<i>b</i> (Å)	7.9388(12)	16.7115(12)	21.821(4)
<i>c</i> (Å)	14.0823(15)	20.5114(15)	7.791(8)
α (°)	76.05	90.00	90.00
β (°)	83.41	90.00	102.53
γ (°)	86.26	90.00	90.00
<i>Z</i>	2	8	4
<i>V</i> (Å ³)	786.52(18)	3319.4(5)	1189.8(12)
<i>D_{calc}</i> (g cm ⁻³)	2.310	2.189	2.562
μ (mm ⁻¹)	2.531	2.399	3.319
<i>F</i> (000)	532.0	2128.0	880.0
No. of unique reflections	6776	43448	10132
No. of observed reflections [<i>I</i> > 2 σ (<i>I</i>)]	3062	3250	2333
Parameters	237	237	174
Goodness-of-fit (GOF)	0.945	1.000	1.051
Final <i>R</i> indices [<i>I</i> > 2 σ (<i>I</i>)] ^{a,b}	<i>R</i> ₁ = 0.0434, <i>wR</i> ₂ = 0.0913	<i>R</i> ₁ = 0.0283, <i>wR</i> ₂ = 0.0629	<i>R</i> ₁ = 0.0293, <i>wR</i> ₂ = 0.0579
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0640, <i>wR</i> ₂ = 0.1068	<i>R</i> ₁ = 0.0317, <i>wR</i> ₂ = 0.0645	<i>R</i> ₁ = 0.0378, <i>wR</i> ₂ = 0.0642
Largest difference peak and hole (e Å ⁻³)	0.78 and -1.06	0.47 and -0.62	0.89 and -1.09

^a $R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|$.

^b $wR_2 = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2]^{0.5}$.

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