

Syntheses and Crystal Structure of Zinc(II) Complex Constructed from taurine Schiff Base

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Abstract: The complex $[\text{Zn}(\text{C}_8\text{H}_9\text{N}_2\text{O}_3\text{S})(\text{C}_8\text{H}_6\text{O}_5)(\text{H}_2\text{O})]$ ($\text{C}_8\text{H}_9\text{N}_2\text{O}_3\text{S}$ = the Schiff base formed by 2-Pyridinecarboxaldehyde and taurine) was synthesized by reaction of $\text{Zn}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$. The crystal structure of the Zinc(II) complex has been determined and studied by X-ray diffraction. The complex is monoclinic, space group $P2(1)/c$, with $a = 10.184(1) \text{ \AA}$, $b = 9.571(2) \text{ \AA}$, $c = 11.637(8) \text{ \AA}$, $\alpha = 81.91(9)^\circ$, $\beta = 85.23(4)^\circ$, $\gamma = 78.56(9)^\circ$, $V = 1134.27(6) \text{ \AA}^3$, $Z = 1$. The asymmetric unit is comprised of a coordination cation together with a mononuclear coordination anion and two water molecules, all of which are linked by hydrogen bonding and π - π interactions into a three-dimensional framework.

Introduction

Taurine is a kind of beta amino acids, which is containing sulfur group. Its unique physiological and pharmacological functions determine its wide application in medicine, food, chemical industry and so on. Schiff base and its complexes have good biological activity, and are attractive to researchers for their attractive prospects in catalysis, biological simulation and analytical chemistry.

In recent years, transition metal complexes of sulfur Schiff base have become one of the focuses for the good antitumor, antibacterial and other physiological activities and catalytic activity. In living organisms, the trace elements, such as, copper and nickel, often in high concentration of biological ligands in the environment, often with more than two kinds of biological ligands to form complexes, plays an important role in catalysis, material transfer process of these complexes in the life process of the enzyme and the storage and transport of metal ions.

Schiff base is a kind of important biological ligand that contains many coordination atoms. The transition metal complexes of Schiff base are similar to macrocyclic ligands. The biological activities of complexes of Schiff base, such as carrying oxygen, antibacterial and good catalytic performance, which has important significance in the fields of biology and medicine, has attracted the interest of researchers. The synthesis of transition metal complexes of Schiff base by traditional chemical methods has been reported, but the yield is not high and the process is complicated. The transition metal Schiff base complexes with friendly environment, high yield, simple operation and one-step synthesis have been shown to be of high value in theory and application, and have always been the synthetic direction that people have been trying to develop.

Experimental

Materials and physical measurements

All solvents and chemicals purchased from commercial sources were of reagent grade and used without further purification. IR spectra were performed on a Shimadzu spectrum FT-IR spectrometer with KBr pallets in the range of $4000 \sim 400 \text{ cm}^{-1}$. The elemental analyses for C, H, N and S were carried out on a Leeman elemental analyzer. The crystal data were collected on a Rigaku Xtalab area detector diffractometer at room temperature.

Synthesis of the ligand(L)

The ligand (L) was prepared as previously reported. 2-Pyridinecarboxaldehyde (10mmol, 1.071 g) was

dissolved in 10 mL absolute methanol, followed by dropping a solvent of taurine (10mmol, 1.251g) and potassium hydroxide (10 mmol, 0.561g) in absolute methanol solution (30mL), and then the mixture was stirred at room temperature. After 2 hours' reaction, a large amount of yellow deposition was generated. After vacuum filtration, the residues were washed with the absolute ethanol 5mL twice, and anhydrous ether 5mL twice. The wet product was dried by vacuum oven, yielding the yellow power compound (H₂L). Yield: 71.3%. Anal. Calcd. (%) for C₈H₉NO₃SK:C 30.09, H 3. 57, N 12. 14, S 12. 56; Found(%): C 31. 15, H 3. 35, N 11. 93, S 12. 87.

Synthesis of complex1

an aqueous solution containing (5mL) Zinc acetate dehydrate (1mmol, 0.220g) was added to the H₂L (1mmol, 0.253g) aqueous solution (10mL) with the proportion of meth 50%. It takes 2hours to reaction at the room temperature, then dropped the methanol solvent (5mL) of 3,5-dihydroxybenzoic acid (1mmol, 0.154g). After stirring for 2 h, the resulting solution was kept at room temperature by slow evaporation for about 9 days, yielding colorless square single crystals. Yield: 36%. Selected IR data (cm⁻¹): (S=O) 1256.5 cm⁻¹ and 1131.1 cm⁻¹, (S–O) 998.2 cm⁻¹ and (C=N) 1608.5 cm⁻¹. Anal. Calcd. (%) for C₁₆H₁₇ZnN₂O₉S: C, 46.08; H, 2.68; N, 4.13; S, 9.46. Found (%): C, 46.11; H, 2.66; N, 4.11; S, 9.48.

Structure determination

A suitable single crystal of complex1 (0.36mm × 0.24mm × 0.11mm) was selected and glued on the tip of a glass fiber. The crystal structure was determined at 298K on an X-ray diffractometer, a Rigaku Xtalab detector diffractometer by using a CuK α radiation ($\lambda = 0.154\text{\AA}$). All structures were solved using direct methods with SHELXS and refined by full-matrix leastsquares on F^2 using the SHELXL14 software within OLEX2. All the non-hydrogen atoms were refined anisotropically with displacement parameters. The hydrogen atoms were generated geometrically and treated by a mixture of independent and constrained refinement using a riding model. Crystal data and structure parameters for the title complex are listed in Table 1.

Table 1 Crystal data for Zinc(II) Compound

Polymers	Complex1
Formula	C ₁₆ H ₁₇ ZnN ₂ O ₉ S
Formula weight	478.52
Temperature(K)	298
Wavelength(A)	0.154
Crystal sizes(mm)	0.36mm × 0.24mm × 0.11mm
Color	colorless
Crystal system	monoclinic
Spaces group	P 2(1) /c
a(A)	10.184 (1)
b(A)	9.571(2)
c(A)	11.637(8)

Table 2 elected Bonds Lengths (nm) and Bonds Angles(°)

Bond Lengths				Bond Angles			
Zn1-O1w	1.925(1)	C1-N1	1.316(2)	O6-Zn1-O1w	90.3(1)	C1-N1-C5	101.9(5)
Zn1-O6	1.924(4)	C7-N2	1.567(1)	N2-Zn1-O1w	98.4(5)	N1-C1-C2	106.3(5)
Zn1-N1	1.851(7)	C6-N2	1.339(6)	N1-Zn1-N2	83.7(2)	N1-C5-C6	110.4(1)
Zn1-N2	2.012(3)	C5-N1	1.326(2)	O6-Zn1-N1	86.9(6)	C6-N2-Zn1	118.9(1)
Zn1-N1	1.845(6)	S1-O1	1.354(5)	O1-S1-O2	112.3(2)	C10-C9-O6	115.6(3)
Zn1-N2	1.672 (5)	S1-O2	1.376(2)	O1-S1-O3	114.2(8)	C9-O6-Zn1	109.6(7)
		S1-O3	1.315(1)	O2-S1-O3	111.7(4)	O7-C9-O6	118.6(2)

Symmetry transformations used to generate equivalent atoms: #1: -x+1, -y+1, -z+1

Results and Discussion

Structural Description

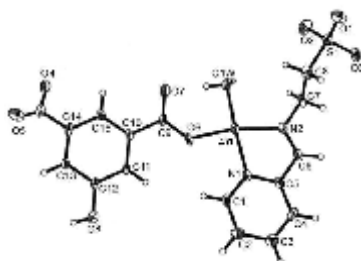


Fig.1 Crystal Structure of complex1 [Zn(C₈H₉N₂O₃S)(C₈H₆O₅)(H₂O)]

X-ray diffraction results show that crystal structure of the complex1. It indicates the central Zinc (II) coordinates two atoms of N (N 1 and N 2) from Schiff base L respectively, oxygen(O6) from the carboxyl of 5-Hydroxyisophthalic acid, and oxygen(O1w) from water. The coordination modes and structural topologies give rise to some valuable information. As shown in Fig1, four coordination atoms, N1, N2, O6 and O1W are almost in the same plane. The angles of the four atoms are O6-Zn1-O1W 90.3(1)°, O1W -Zn1-N2 98.4(5)°, N2 -Zn1-N1 83.7(2)°, N1 -Zn1-O6 86.9(6)°. The sum of the four angles nearly 359.3°, which reveals that coordinated atoms in the same plane.

IR Analysis

The infrared spectra of ligands and coordination polymers were determined by the potassium bromide tableting method in the range of 4000 - 400cm⁻¹ wavenumbers. There are strong peaks which were found near the 1621 cm⁻¹. It indicates the formation of C=N Schiff base. The absorption peaks of 1189 cm⁻¹ and 1008cm⁻¹ are characteristic absorption peaks of sulfonic group. We also find absorption peaks at 1294 cm⁻¹ which belong to C - O of phenol oxygen. The absorption peak at 1442cm belongs to the benzene. The absorption peaks found around 831cm⁻¹ and 738cm⁻¹ belong to the characteristic absorption peaks of pyridine. It is obviously that -OH stretching frequency of water molecules coordinate because of the presence of the broad band around 3430 cm⁻¹. Comparison with the infrared spectra of the ligand and the synthesized Zinc complex, it makes clear that the coordination bonds have formed.

Thermal Stability Behavior

In order to discuss the thermal stability of the Zinc complex, the thermogravimetric analysis of the Zinc complex is carried out under conditions of temperature with the increasing rate 10°C/min, from 25°C to 450°C. There are two steps of the decomposing. Thermal analysis of complex shows that the weight loss starts at 56-66°C, the total loss of 3.607% attributed to the release of H₂O, which is calculated 3.762%. The exquisite weight loss appears at 346-389°C, which is attributing to the decomposing of the Schiff base. The final residues is comparing with other complexes which are depending on the bridging ligands, the network structure constructing with chelating ligands is relatively unstable.

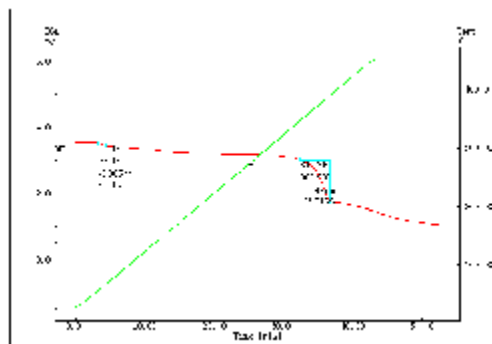


Fig.2 The thermogravimetric analysis of the Zinc complex

Conclusions

In this paper, we have presented the Zinc(II) complex $[Zn(C_8H_9N_2O_3S)(C_8H_6O_5)(H_2O)]$ ($C_8H_9N_2O_3S$ = the Schiff base synthesized by 2-Pyridinecarboxaldehyde and taurine). The crystal structure of the Zinc (II) complex has been determined and studied by X-ray diffraction, which is also characterized by elemental analysis, IR spectra. Thermogravimetric analysis also has been studied in order to investigate the thermal behavior carefully.

Acknowledgements

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