Synthesis and Structure of Zinc Complex of N, N-bis (benzimidazol-2-yl-methyl) amine

Xiao Lan LIU*, Qing Yan CHENG, Xia YANG, Zhi Wei MIAO, Wei LIU
Fang Ming MIAO

College of Chemistry and Life Science, Tianjin Normal University, Tianjin 300074

Abstract: The Zinc complex of N, N-bis (benzimidazol-2-yl-methyl)amine has been synthesized and its crystal structure determined by X-ray diffraction method. The structure features of the complex are described.

Keywords: Zinc compex, N, N-bis (benzimidazol-2-yl-methyl)amine, superoxide dismutase (SOD)

Histidine is known to be an important biological ligand present at the active site of superoxide dismutases (SOD)[1-2] and other metalloproteins. It appears to play a crucial role in the coordination chemistry of numerous metalloproteins. The ligand of di(2-benzimidazolyl-methyl)amine (L3) was chosen as the model compound of histidine. This paper reports the synthesis and crystal structure of Zn-L3 complex which is as the model compound of SOD.

The complex, $Zn(L3)_2\cdot(ClO_4)_2\cdot C_2H_5OH$($C_{32}H_{30}N_{10}Zn\cdot(ClO_4)_2\cdot C_2H_5OH$) (obs. %: C 47.42, H 4.16, N 16.45; calc.%: C 47.21, H 4.20, N 16.20), was characterized by means of IR, UV and X-ray single crystal diffraction. IR(KBr, cm^{-1}) 1624(C = C), 1454, 1470 (C = N**(**imidazole**)**), 1275(C-N**(**imidazole**)**), 1336(C-N**(**alkylamine**)**). UV: 214, 243, 273, 279 nm. The crystal structure was solved by direct method *MULTAN82* program. The perspective drawing of the coordinated ion$[Zn(L3)_2]^{+2}$ of the complex is shown in **Figure 1.** The crystallographic data are as follows: triclinic system, space group $P\text{-}1$, a = 12.027(2), b = 12.353(2), c = 15.298(3)Å, α = 80.76(3), β = 86.55(3), γ = 68.04(3)°, V = 2081(1) $Å^3$, Z = 2, R = 0.072, R_w = 0.077.

The crystal structure of the complex shows that one stoichiometric molecule is composed of one $[Zn(L3)_2]^{2+}$, two $(ClO_4)^-$ and one C_2H_5OH molecule. Two alkylamino N atoms and four 4-position N atoms of imidazolyls from two ligands are coordinated to zinc ion to form a distorted octahedron geometry which is similar to the structure of $C_{32}H_{30}N_{10}Cu\cdot(ClO_4)_2\cdot H_2O$[3]. The bond angle of N1-Zn-N9, N2-Zn-N5, and N3-Zn-N7 are 164.4, 164.1 and 162.9° respectively. The largest deviation of Zn^{2+} from the equatorial plane is 0.26 Å.

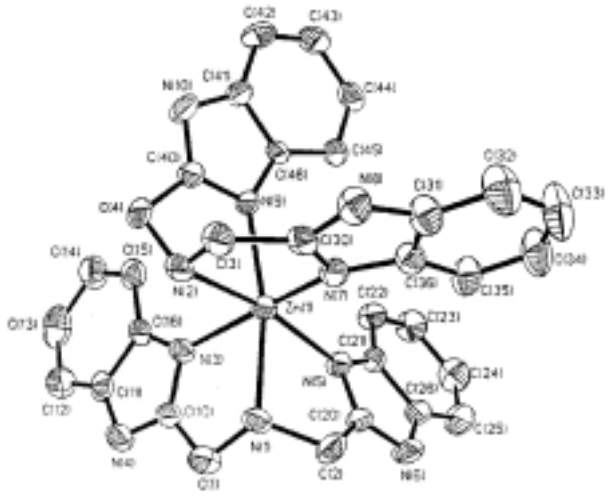
The activity of this kind of bi-ligand complex is lower than that of mono-ligand complex[4]. This result shows that in order to increase the biological activity of SOD

model compounds, the center metal irons should possess the complexed sites for the weak complexing groups, particularly for $O_2^{-\bullet}$radical, to attack the center metal irons.

Experimental

A mixture of *o*-phenyldiamine (0.2 mol) and imino-acetic acid (0.1 mol) in glycol was refluxed for 24 h. After cooling, 500 ml water was added and 10% NaOH was dropped in with stirring to PH ≈ 8, then filtered and washed the precipitate with water, white powder of [di(2-benzimidazolyl-methyl)amine(L3)] was obtained. A mixture of L3 (4 mmol) and $Zn(ClO_4)_2 \cdot 6H_2O$ (2 mmol) in ethanol was stirred for 3 h at the room temperature, then distilled ethanol and cooled, the light-yellow powder obtained was recrystallized from ethanol. The single crystal structure of the complex $Zn(L3)_2(ClO_4)_2 \cdot C_2H_5OH$ was determined on an Enraf-Nonius CAD-4 diffractometer with graphite-monochromated Mo Kα radiation (λ = 0.71073Å).

Figure 1 The perspective drawing of the coordinated ion $(C_{32}H_{30}N_{10}Zn)^{+2}$ of the title complex



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References and note

1 Y. Kitagawa, N. Tanaka, Y. Hata, et al., J. Biochem., **1991**, 109, 477.
2 J. B. Cooper, H. P. C. Driessen, S. P. Wood, *et al., J. Mol. Biol*., **1994**, *235*, 1156.
3. M. Palaniannda var, T. Pandiyan, M. Lakshminarayanan, *et al., J. Chem.Soc.Dakton Trans*., **1995**,455.
4. Q.Y. Cheng, *A dissertation for the degree of Master*，Tianjin Normal University，**1998**.
5. The crystallographic parameters of the compound have been deposited in the editorial office of CCL.

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