

SHORT COMMUNICATION

NEW HALOTIN (IV) WITH EDTA: SYNTHESIS AND INFRARED STUDY

Serigne Cissé, Ibrahima Cissé, Libasse Diop*

*Université Cheikh Anta Diop, Faculté des Sciences et Techniques,
Département de Chimie, Laboratoire de Chimie Minérale et Analytique
(LACHIMIA), Dakar, Sénégal*

*Corresponding author: dlibasse@gmail.com

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Abstract: Tri acidic or neutral ethylenediaminetetraacetato [H_3Y^- or Y^{4-}] containing adducts and derivatives have been synthesized and studied by infrared. The suggested structures are discrete with octahedral environments around the tin centres, the ethylenediaminetetraacetic anion behaving as a tridentate, pentachelating and bidentate, pentachelating and tridentate ligand. For the last structure when intermolecular hydrogen bonds involving OH group are considered, a supramolecular architecture may be obtained.

Keywords: *discrete structures, ethylenediaminetetraacetic anion, hydrogen bonds, pentachelating and bidentate, pentachelating and tridentate, supramolecular architectures*

INTRODUCTION

The interesting structural aspects and applications in organotin (IV) chemistry- medicine, agriculture, industry- explain the interest of various research groups worldwide [1- 4]. In the framework of our research work in the coordinating ability of oxyanions towards organotin(IV) molecules, our group has yet published some papers [5-10] and report here the study of the interactions between $[\text{Me}_4\text{N}][\text{H}_3\text{Y}]\cdot\text{H}_2\text{O}$ or $[\text{BzNMe}_3]_2[\text{H}_2\text{Y}]\cdot\text{H}_2\text{O}$ and SnCl_2 which has yielded tri new compounds, infrared study of which have been carried out then structures suggested on the basis of spectroscopic data.

MATERIALS AND METHODS

$[\text{Me}_4\text{N}][\text{H}_3\text{Y}]\cdot\text{H}_2\text{O}$ (L_2) and $[\text{BzNMe}_3]_2[\text{H}_2\text{Y}]\cdot\text{H}_2\text{O}$ (L_5) have been obtained as powders after the water evaporation of the solution obtained on dissolving ethylenediaminetetraacetic acid (EDTA) in aqueous solutions of Me_4NOH or BzNMe_3OH in 1:4 ratio. The analytical data % calculated (% found): (L_2): C = 43.86 (43.14), H = 7.62 (7.27), N = 10.96 (10.33); (L_5): C = 59.19 (59.07), H = 7.95 (7.87), N = 9.20 (9.23) have allowed to suggest the above formulae for (L_2) and (L_5).

When SnCl_2 are allowed to react with (L_2) and (L_5) in ethanol in specific ratios, white precipitates are obtained which are stirred around two hours and washed with ethanol:

- SnCl_2 with L_2 in 3:1 ratio gives (**A**);
- SnCl_2 with L_5 in 3:1 ratio gives (**B**);
- SnCl_2 with L_5 in 6:1 ratio gives (**C**);

The analytical data have allowed to suggest the following formulae for the three new compounds (Table 1):

Table 1. Suggested formulae of the synthesized compounds

| Comp | Suggested formulae | Chemical composition [% mass] | | | | | |
|----------|---|-------------------------------|-------|-------|-------|-------|-------|
| | | C | | H | | N | |
| | | Calc. | Found | Calc. | Found | Calc. | Found |
| A | $(\text{Me}_4\text{N})_4\text{Y}\cdot 2\text{SnCl}_4\cdot\text{SnCl}_3\text{Me}_4\text{N}\cdot 2\text{H}_2\text{O}$ | 23.83 | 23.72 | 5.07 | 4.70 | 6.48 | 6.35 |
| B | $\text{SnY}\cdot 3/2\text{SnCl}_2(\text{OH})_2\cdot\text{H}_2\text{O}$ | 16.14 | 16.23 | 2.25 | 2.32 | 3.68 | 3.42 |
| C | $\text{SnY}\cdot 5/2\text{SnCl}_2(\text{OH})_2\cdot\text{EtOH}\cdot 2\text{H}_2\text{O}$ | 13.75 | 13.54 | 2.60 | 2.87 | 2.67 | 2.35 |

The infrared spectra were recorded with a Bruker FTIR (4400 -350 cm^{-1}) spectrometer at Saint Boniface College, Winnipeg-Canada. The elemental analyses have been performed at the laboratory of Microanalyses at the University of Bath (UK). Infrared data are given in cm^{-1} [IR abbreviations: (br) broad, (vs) very strong, (s) strong, (m) medium, (sh) shoulder]. All the chemicals are from Aldrich Company (Germany) and were used without any further purification.

RESULTS AND DISCUSION

Let us consider the infrared data of the studied derivatives based on assignments in [11]:

A: $\nu(\text{OH}_2) = 2925 \text{ s}$; $\nu_{\text{as}}(\text{COO}) = 1500 \text{ s}$; $\delta(\text{CH}_2) + \nu_{\text{s}}(\text{COO}) = 1458 \text{ s}, 1376 \text{ s}$; $\nu(\text{CC}) = 774 \text{ s}$;

B: $\nu(\text{OH}_2) = 3066 \text{ sh}$; $\nu_{\text{as}}(\text{COO}) = 1626 \text{ s}, 1599 \text{ s}$; $\delta(\text{CH}_2) + \nu_{\text{s}}(\text{COO}) = 1457 \text{ s}, 1305 \text{ sh}$; $\nu(\text{CC}) = 722 \text{ m}$;

C: $\nu(\text{OH}_2) = 3064 \text{ s}$; $\nu_{\text{as}}(\text{COO}) = 1667 \text{ s}, 1621 \text{ s}$; $\delta(\text{CH}_2) + \nu_{\text{s}}(\text{COO}) = 1377 \text{ m}$; $\nu(\text{CC}) = 774 \text{ m}$.

From these data we suggest three discrete structures with the ethylenediaminetetraacetic anion behaving as a tridentate, pentachelating and bidentate, pentachelating and tridentate the environments around the tin centres being octahedral.

For **A** a discrete structure with octahedral Sn centres, the anion behaving as a tridentate ligand is suggested (Figure 1).

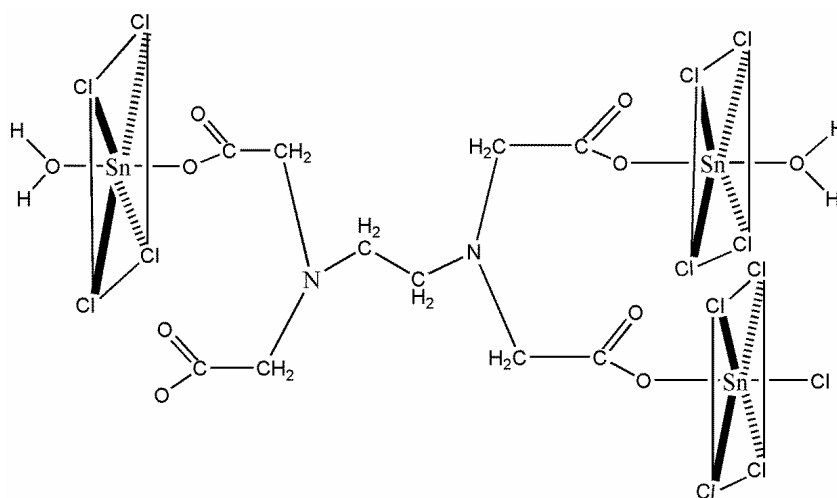


Figure 1. Proposed structure for the compound **A**

For **B** a dimeric structure is suggested with a octahedral environment around Sn centres, the anion behaving as a pentachelating and bidentate ligand, the water molecules as coordinated ones (Figure 2).

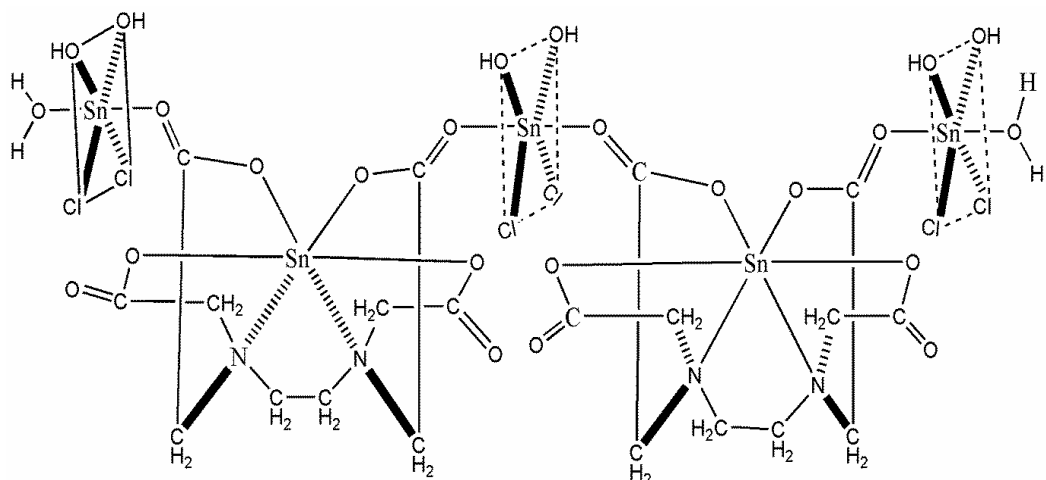


Figure 2. Proposed structure for the compound **B**

For **C** a dimeric structure is suggested with an octahedral environment around Sn centres, the anion behaving as a pentachelating and tridentate ligand, the water molecules as coordinated ones and two EtOH molecules being connected to $[2\text{SnY}\cdot 5\text{SnCl}_2(\text{OH})_2\cdot 4\text{H}_2\text{O}]$ through OH---O hydrogen bonds (Figure 3).

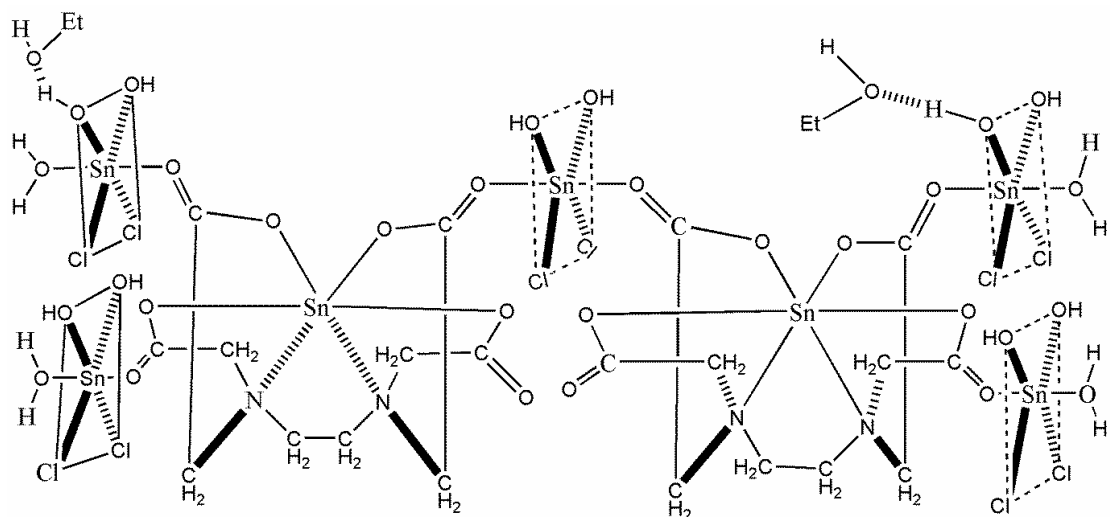


Figure 3. Proposed structure for the compound **C**

For the last structure when extra hydrogen bonds are considered supramolecular architectures may be obtained.

CONCLUSIONS

The structures of three compounds studied in this work have a discrete structure with octahedral environments around the tin centres, the anion behaving as a tridentate, pentachelating and bidentate, pentachelating and tridentate ligand. For the last structure when intermolecular hydrogen bonds are considered involving OH group, a supramolecular architecture may be obtained.

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