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Synthesis, structure and biological ability of organotin carboxylate derived from modified amino benzo thiazole

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A novel ligand, 2-[(1,3-benzothiazol -2-yl) amino] acetic acid (BAA), has been prepared by condensation reaction of 2-aminobenzothiazole with chloroacetic acid. BAA prepared ligand has been applied to prepare three different organotin carboxylate complexes *via* condensation reactions with a salt of corresponding organotin(IV) chloride. The synthesized ligand BAA and complexes have been systematically identified *via* the use of Fourier transform infrared spectroscopy (FTIR), multinuclear magnetic resonance spectroscopy (^{1}H and ^{119}Sn NMR), and carbon (C), hydrogen (H) and nitrogen (N) elemental analysis, checking their fundamental integrity. BAA antioxidant ability and their organotin(IV) carboxylate complexes have been estimated *via* different established methods: CUPRAC (Cu ion Reducing Antioxidant Capacity) and DPPH (2,2-diphenyl-1-picrylhydrazyl) radical scavenging assays. Results point towards all organotin(IV) carboxylate complexes showing significantly larger inhibition percentages in contrast to free BAA ligand, underlining the serious role of the Tin(IV) centers in raising antioxidant ability. Particularly, the $Ph_3Sn(IV)COO$-complex has demonstrated superior functioning by both methods, assigned to its noticeable steric and electronic properties resulting from the Ph_3 group substituents.

Keywords: Ability, Amino benzothiazole, Condensation reaction, Organotin-carboxylate complex

Organotin (IV) carboxylates are a significant class of compounds that have drawn more attention recently due to their many uses as well as their inherent appeal[1,2]. Numerous diorganotin and triorganotin species have been found to exhibit potential as antituberculosis and anti-neoplastic medications in investigations conducted to assess their anti-tumor action[3–5]. Investigating the chemistry of compounds containing indomethacin and (OTs) was deemed interesting due to the pharmacological significance of indomethacin acid, also the possible biological ability of organotin carboxylates. In keeping with our research on biological organotin chemistry, coordination chemistry, and the anti-inflammatory qualities of NSAIDs like tyrosine, ampicillin and cephalexin[6–9]. Generally, tri-OTs (IV) complexes have a wider range of biological activity compared to their mono- and di-organotin counterparts[10]. Their capacity to bind proteins has been ascribed to this[11]. Additionally, it was discovered that numerous organotin (IV) carboxylates exhibited anticancer properties in a range of tumor cells, solid-phase and solution-phase configration of these organotin (IV) compounds were described [JMCS][12]. Here, we describe the synthesis and spectrum analysis of BAA and the resulting complexes. The complexes have been structurally studied in solution using ^{1}H NMR spectroscopy and in the solid state applying ^{119}Sn Mossbauer and vibrational spectroscopy (Fig. 1, Fig. 2 and Fig. 3). Additionally, the biological activity of BAA and its derivative complexes was investigated using various techniques.

Experimental Section

Preparation of Ligand BAA

By reacting a suitable amount of material, the ligand was created. 2- Aminobenzothiazole (0.15 gm, 1 mmol) and (0.094 gm, 1 mmol) of chloroacetic acid were combined in a methanolic solution and agitated for approximately half an hour at RT. Filtration and drying were performed on the pink ligand (BAA) precipitate.

Preparation of Triphenyl tin(IV) Complex 1

At RT for about 30 minutes, the produced ligand (BAA) in a solution of methanol (1 mmol, 0.21 gm)

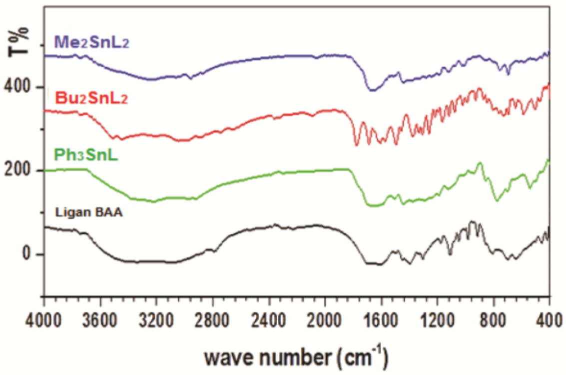

Fig. 1 — FTIR Spectra of BAA and its complexes

was agitated with (1 mmol, 0.4 gram) sodium hydroxide. After dissolving a (1 mmol, 0.385gram) of triphenyl tin chloride (Ph_3SnCl) in 30 mL of hot methanol, it was added to the BAA ligand and allowed to reflux for approximately 4 hours while being constantly agitated[13–15]. After being vacuum-evaporated, the pale purple precipitate was cleaned with diethyl ether and allowed to dry.

Preparation of di-Butyl or Methyltin(IV) Complexes 2-3

For 30 minutes at RT, a 30 mL methanolic solution of the produced ligand (BAA) (2 mmol, 0.30 gram)

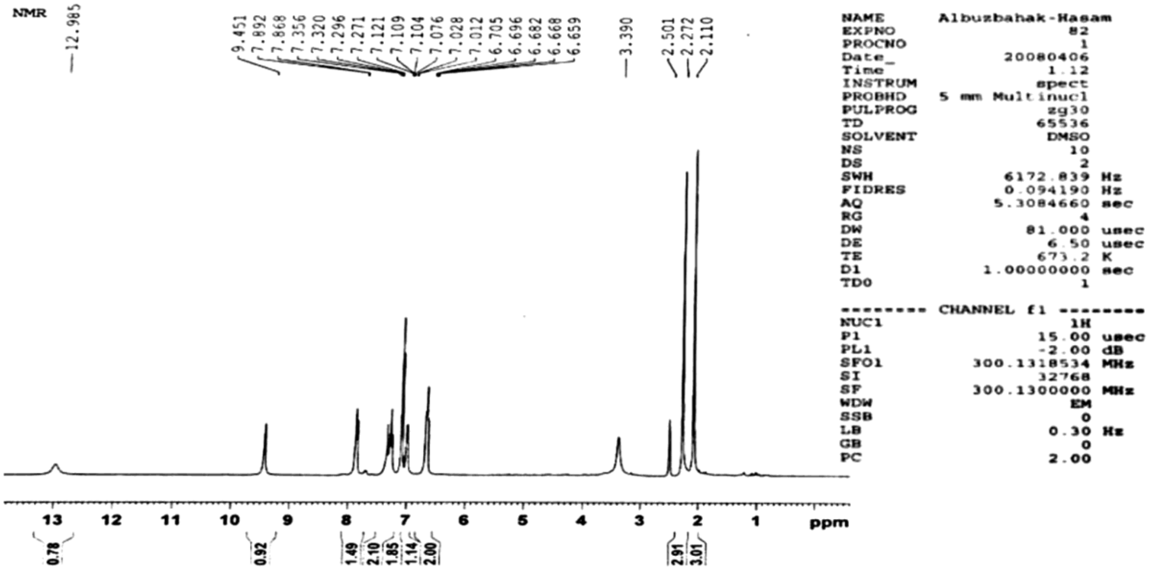

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Fig. 2 — ^{1}H NMR of BAA

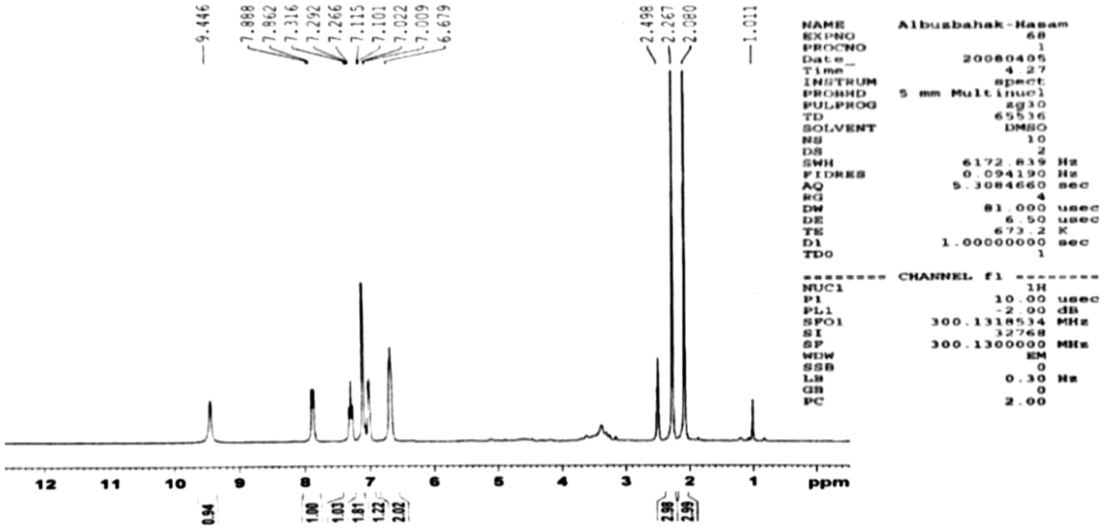

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Fig. 3 — ^{1}H NMR of Bu_2Sn-BAA

was combined with 2 mmol, 0.8 gram of sodium hydroxide. 20 mL of hot methanol was used to dissolve 1mmol, 0.303gm, or 0.22gm of di-n-butyltin or dichlodimethyltin (Bu_2SnCl_2 or Me_2SnCl_2), which was added then to the (BAA) mixture and permitted to reflux for four hours while being constantly stirred[16–19]. After being vacuum-evaporated, the dark pink and brown precipitates were cleaned with diethyl ether and allowed to dry.

Antioxidant Activity Tests

DPPH technique

Using the 1,1-di phenyl-2-picrylhydrazine (DPPH) technique, antioxidant activity was determined. MeOH was used to dissolve the chemical at certain concentrations ranging from 2 to 32 M. The test miture can be carefully mixed with a solution of 0.1 mM DPPH in MeOH. The combination was a waste after half an hour. Using a UV-vis spectrophotometer to measure the mixture's absorbance at (Λ_{max} = 517 nm)[20,21]. Equation (1) was used to measure the inhibition percentage.

$$\textit{Inhibition}\% = (\textit{Absorbance Control} - \textit{Absorbance of Sample}) \times (\textit{Absorbance Control})^{-1} \times 100 \quad \ldots (1)$$

CUPRAC Method

CUPRAC method was applied as another technique to investigate an antioxidant ability[22].

$$\textit{Total antioidants levals} = \left[\frac{A\ test}{A\ STD}\right] \times \textit{Conce. of STD}\left(\frac{mmole}{L}\right) \quad \ldots (2)$$

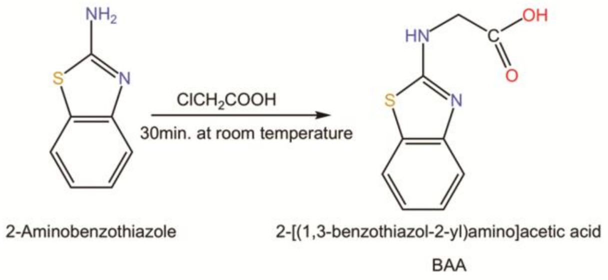
Results and Discussion

Preparation of ligand BAA

The synthesis of the preparation of new ligand BAA was expressed in Fig. 4, *via* stirring 2-aminobenzothiazole with 2-chloroacetic acid about half an hour and in the RT. Scheme 1 demonstrates the synthesis of the new ligand BAA.

Synthesis of BAA - Organotin(IV) Complexes 1–3

By refluxing the ligand BAA in methanolic solutions with tri and di-organotin chloride, the new complexes of Triphenyltin-BAA, di-butyltin$(BAA)_2$, or dimethyltin$(BAA)_2$ were produced, yielding a high percentage from complexes (Scheme 2 and Scheme 3).



Scheme 1 — Synthesis of the new ligand BAA

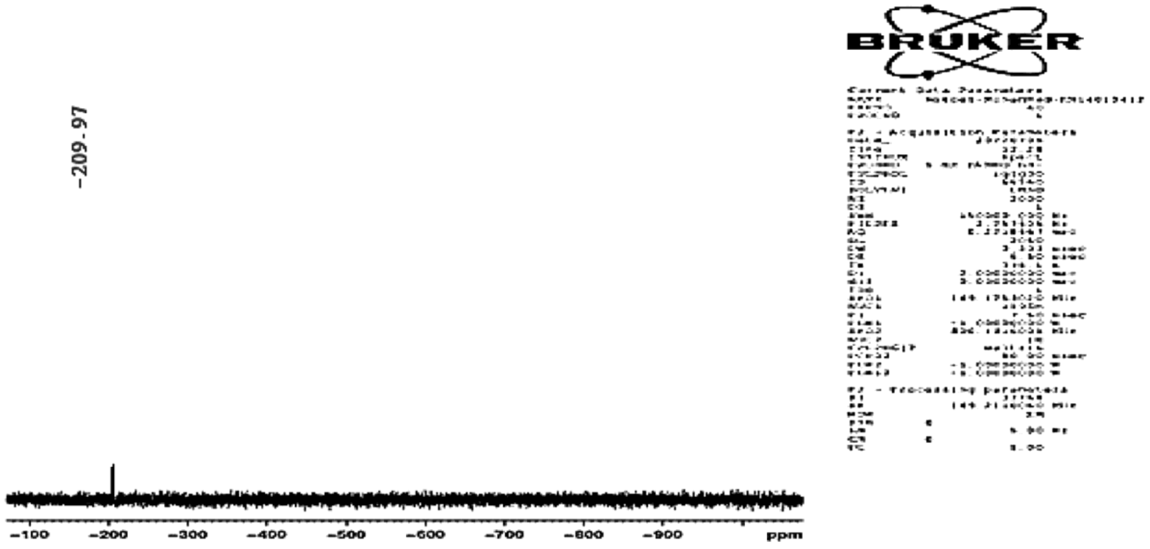
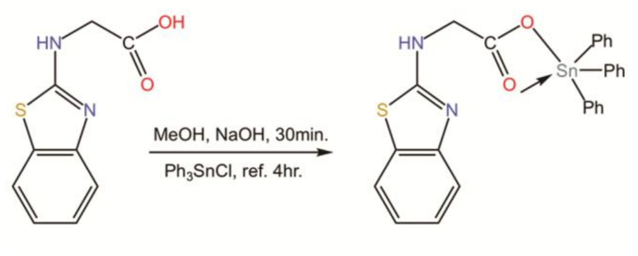


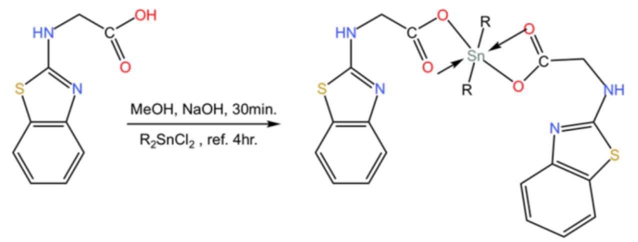
Fig. 4 — ^{119}Sn NMR of $Me_2Sn(BAA)_2$

Along with elemental studies, the resultant compounds were characterized utilizing a variety of techniques, such as FTIR and NMR (^{1}H and Sn^{119}) spectroscopy approaches. The outcomes of each strategy are reviewed in Table 1, Table 2 and Table 3.

IR spectral data of BAA distinguish by existence of amino group absorption at 3430-3321 cm^{-1}. At 3000-2900 cm^{-1}, the CH stretching frequency absorbs. The carboxyl group was visible as a wide band between 2500 and 3100 cm^{-1}. Complexation caused all of these bands to shirt. At 520-515cm^{-1} and 450-445 cm^{-1} absorption bands related to Tin-Oxygen band Tin-Nitrogen band respectively.



Scheme 2 — Synthesis of Ph$_3$Sn(BAA) complex 1



Scheme 3 — Synthesis of Bu$_2$Sn(BAA)$_2$ and Me$_2$Sn(BAA)$_2$

^{1}H NMR At 7.21–7.47, the spectrum displays changed signals associated with the benzene ring. In addition, the NH-group was at 9.45, and N-methyl was at 2.69–2.78. The complexation caused these signals to change. ^{1}H NMR results are expressed in Table 3. The ^{119}Sn NMR was examined for the produced compounds in order to determine their geometrical shape. If the ^{119}Sn NMR value less than 200 its said that complex has 5 coordination structure, if this value appeared at range larger than 200, an octahedral structure, this implies six coordination complex was postulated[23].

The ^{119}Sn NMR spectra of the Ph$_3$Sn(BAA), Bu$_2$Sn(BAA)$_2$, and Me$_2$ Sn(BAA)$_2$ complexes, show singlet signals at the (-180, -256, and -209) ppm area. The chemical shift is determined by the complexes geometry, and these changes are consistent with the idea that the coordination number of the complexes tin atom has increased. Bu$_2$SnCl$_2$ and Me$_2$SnCl$_2$ have octahedral geometry, but the Ph$_3$SnL complex possesses trigonal bipyramidal geometry[16,17].

Table 1 — BAA physical analysis data with complexes

Compd	Colour	Yield (%)	m.p. (°C)	Elemental analysisCalculated (%) (Found)		
				C	H	N
Ligand BAA	Pink	93.2	127-129	50.57(51.06)	6.13(6.71)	32.18(32.93)
Ph$_3$SnL	Purple	90.5	180-182	63.85(64.15)	11.55(12.21)	15.41(15.43)
Bu$_2$SnL$_2$	Brown	92.6	218-210	28.67(28.92)	4.65(5.22)	10.56(10.97)
Me$_2$ SnL$_2$	Dark pink	94.3	222-224	24.76(25.13)	3.81(4.21)	13.33(14.01)

Table 2 — FT IR: BAA and its complexes' spectral data

Compd	NH	C=O	C=C	M-O	M-N
BAA	–	1652	1590	–	–
Ph$_3$- BAA	3406-3323	1643	1572	520	450
Bu$_2$ (BAA)$_2$	3407-3328	1647	1591	514	445
Me$_2$ (BAA)$_2$	3405-3324	1645	1589	515	443

Table 3 — ^{1}H and ^{119}Sn NMR of BAA and compounds spectra

Compd	^{1}H NMR (δ)	^{119}Sn NMR (δ)
BAA	12.98 (s, COOH, 1proton), 9.451 (s, NH, 1proton), 7.21-7.97(m, 5proton, Ar-proton), 2.70-2.78(s, 3 proton, N-methyl).	–
Ph$_3$ BAA	9.55 (s, NH), 7.26-7.50 (m, 5 proton, Ar. proton), 7.55-7.78(m, 5 proton, phenyl group), 2.82(s, 3 proton, N-methyl).	–180
Bu$_2$ (BAA)$_2$	8.08(s, 1proton, NH), 7.23-7.45(m, 5 proton, Ar. proton), 2.69-2.78(s, 3 proton, N-methyl), 0.83-1.59(m, 18 proton, 2 butyl groups).	–256
Me$_2$ (BAA)$_2$	9.5(s, proton, NH), 6.21-7.95(m, 5 proton, Ar. proton), 2.37-2.96(s, 3 proton, N-methyl), 0.80-1.23(s, 6 proton, 2methyl groups)	–209

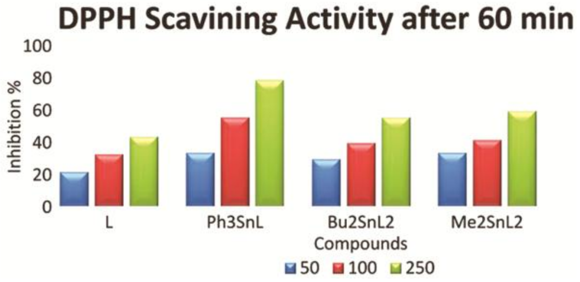


Fig. 5 — Ability of DPPH for BAA and complexes

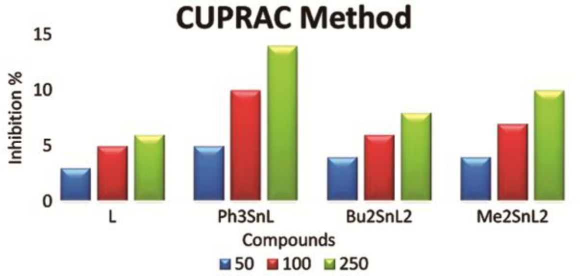


Fig. 6 — CUPRAC Method for BAA and complexes

Antioxidant Activity

To study the antioxidant activity of the 3 prepared BAA-organotin complexes in different amounts, two different methods were applied. The inhibition % may be studied when the absorbance of each measurement was attained, Fig. 5 and Fig. 6.

All the prepared complexes appeared higher activity than BAA ligand derived from. Triphenyltin-BAA (Complex 1) exhibited higher activity than the other synthesized complexes; this possibly related to the fact that Ph_3Sn-BAA complex has 3 phenyl groups besides, large content of aromaticity as compared with the aliphatic groups of di butyl or dimethyltin complexes.

Conclusion

Three matching organotin (IV) carboxylate complexes with a high yield percentage were generated by the BAA reaction as a novel ligand with di and tri-organotin chloride. BAA and its complexes of organotin(IV) (OTs) antioxidant activity were controlled *via* the use of CUPRAC and DPPH procedures. The BAA derived complexes exhibited higher antioxidant ability from that of the BAA ligand itself. This is may be associated to the existence of different organic groups, besides metal Sn content.

Authors' contribution

AGH, DJ and IJ: Methodology; DJ, AGH and SJB; formal analysis and investigation; AGH and IJ writing and editing; All authors have read and agreed to the published the manuscript.

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