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Novel N-S bond scission and ring-opening reactions upon addition of phosphines to benzisothiozolinate zinc(II) complex

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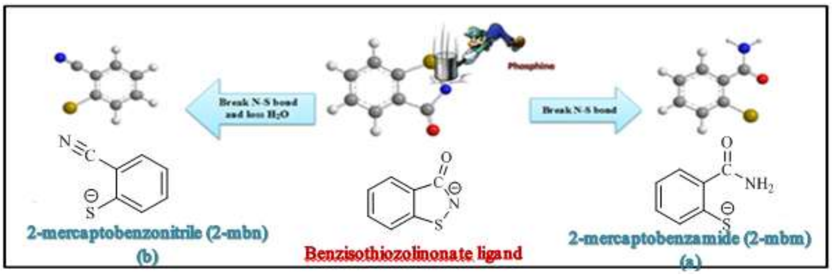
ABSTRACT

Reaction of two equivalents of sodium benzisothiozolinate (Nabit) with one equivalent of zinc acetate in aqueous solution afford $[Zn(bit)_2(H_2O)]_2$ (1). Treatment of (1) with three equivalents of triphenyl phosphine (PPh_3) gave $[Zn(PPh_3)_2(\kappa^1\text{-2-mbm})(\kappa^1\text{-2-mbn})]$ (2), (2-mbm=2-mecaptobenzamide, 2-mbn=2-mercaptobenzonitrile). Treatment of (1) with one equivalent of the bidentate diphoshine ligands (diphos), $Ph_2P(CH_2)nPPh_2$, n = 1 ,(dppm) afforded two polemerization isomers complexes $[Zn(\kappa^1\text{-dppm})(\kappa^2\text{-2-mbm})(\kappa^1\text{-2-mbn})]$ (3a) and $[Zn(\mu\text{-dppm})(\kappa^1\text{-2-mbm})(\kappa^1\text{-2-mbn})]_2$ (3b), when n = 2 (dppe), the product is $[Zn(\kappa^2\text{-2-mbm})(\mu\text{-2-mbn})]$ (4), when n = 3 (dppp), n =4 (dppb) or $(CH_2)n = (C_5H_4)_2Fe$, bis(diphenylphosphino) ferrocene (dppf) afforded complexes of the type $[Zn(diphos)(\kappa^1\text{-2-mbm})(\kappa^1\text{-2-mbn})]$ (5-7).

In all these reactions the N-S bond of the heterocyclic benzisothiozolinonate ring is broken and protonated to produce the 2-mercaptobenzamide ligand (2-mbm), then the product loses H_2O molecule to afford a 2-mercaptobenzonitrile (2-mbn) ligand. The synthesized complexes were characterized by elemental analysis, infrared spectra conductivity measurements and multinuclear ^1H and ^{31}P nmr spectra.

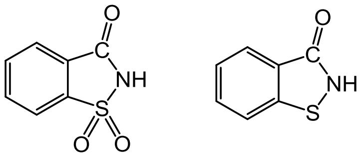


1. Introduction

Saccharin (sacH, 2H-1λ6,2-benzothiazol-1,1,3-trione, is a well-known non caloric artificial sweetener. Saccharin (sacH) has very low solubility therefore, it is employed in the form of sodium saccharinate salt, Na(sac). Saccharinate (sac) has been shown to be a versatile poly-functional ligand with extensive coordination chemistry [1-8]. It has three potential coordination sites, the negatively charged N, carbonyl and sulfonyl oxygens for metal ions and therefore, the coordination chemistry of sac is rich and interesting. It usually coordinates to different metal ions through the negatively charged N atom, but it also displays tridentate chelating and bridging coordination modes, forming a wide range of metal complexes from mononuclear to coordination polymers. While coordination chemistry of saccharinate (sac) has been extensively studied [1], the closely related benzisothiozolinate (bit) ligand remains virtually unexplored [9-12] (Chart 1). Benzisothiozolinate (bit) ligand is poly-functional also, it can bind to metal ions through the negatively charged N, carbonyl or sulfur atom [9-12].

The coordination of Zn(II) ion in a sulfur-ligated environment is a clearly feature of structural and functional sites of many important metalloproteins. Examples of such enzymes include the liver alcohol dehydrogenase [13]. and repair protein [14], the Cobalamine dependent and -independent methionine synthases, and farnesyl-transferase [15].

We recently initiated a systematic study of benzisothiozolinate coordination chemistry and have recently shown that it can bind to Pd(II) as a monodentate ligand through the amide nitrogen [9,10] or as bidentate chelating ligand through the amide nitrogen and oxygen atom of carbonyl group [11,12]. As a continuation to our interest in the coordination chemistry of benzisothiozolinate ligand [9-12], we report here the synthesis of Zn-bit complex and reactivity of Zn-bit complex with mono and diphosphine ligands.



sacH bitH

Chart 1: sacH and bitH ligands

2. Experimental

General methods, reagents and instrumentation

Phosphines ligands, zinc(II) acetate and benzisothiozolinone (Hbit) were commercial products, and used without further purification. Sodium benzisothiozolinate (Nabit) was prepared by literature method [9]. ^{1}H NMR and ^{31}P spectra recorded on a Varian Unity spectrometer–using d^6-DMSO or $CDCl_3$ as solvent. IR spectra were recorded on Shimadzu FT-IR 8400 spectrophotometer in the 400-4000 cm^{-1} range as KBr discs. Elemental analyses were carried out at Ibn-Al-Haitham Lab. University of Baghdad, Iraq, using a CHN-analyzer type 1106 Carlo-Erba.. Melting points measured on a Gallenkamp melting point apparatus and are uncorrected. Conductivity measurements were carried out on 10^{-3} molar solutions of DMSO using a digital conductivity meter.

2.2. Synthesis of complexes

Synthesis of $[Zn(bit)_2(H_2O)]_2$ (1)

An aqueous solution of NaBit (0.515 g, 2.979 mmol) in (10 cm^3) was added with stirring to an aqueous solution of $[Zn(OAc)_2].2H_2O$ (0.326 g, 1.487 mmol) in (15 cm^3), a white precipitate was formed immediately after addition. The mixture was stirred with heating on a water bath for an hour. The white solid formed was filtered off, washed with cooled distal water and dried in vacuum oven at (50 °C). (Yield: 0.833 g, 76%).

Synthesis of $[Zn(PPh_3)_2(\kappa^1$-2-mbm)(κ^1-2-mbn)] (2)

A mixed solvents of ethanol (10 cm^3) and chloroform (10 cm^3) was added to a mixed solid of PPh_3 (0.3631g, 1.368mmol) and **(1)** (0.4502 g, 0.557 mmol) in a molar ratio (3:1) (phosphine : complex) . The mixture was stirred for an hour then refluxed for 4h to afford a clear solution. The reaction solution was filtered off and left to evaporate slowly at room temperature. The white precipitate formed was filtered off, and dried under vacuum. The product was recrystallized from acetone to give white powder (Yield: 0.1983 g, 49%).

Synthesis of $[Zn(\mu$-dppm)(κ^1-2-mbm)(κ^1-2-mbn)]$_2$ (3a)

And $[Zn(\kappa^1$-dppm)(κ^2-2-mbm)(κ^1-2-mbn)] (3b)

Chloroform (10 cm^3) was added to a mixed solid of dppm (0.153 g, 0.399 mmol) and **(1)** (0.146 g, 0.399 mmol) in a molar ratio (1:1) (phosphine : complex) . The mixture was stirred for an hour then refluxed for 4 hours. The resulting clear solution was stirred for 48 hours, then ethanol (10 cm3) was added to the reaction mixture. The mixture was refluxed for 2 hours to afford a colorless solution. The resulting solution was left to cool at room temperature, filtered off and set aside to evaporate slowly. The white precipitate formed was filtered off, and dried under vacuum at 50 °C. The product was recrystallized from acetone to give white powder (Yield: 0.2381 g, 41%).

Synthesis of $[Zn(\kappa^2$-2-mbm)(μ-2-mbn)] (4)

Ethanol (20 cm^3) was added to a mixed solid of dppe (0.171 g, 0.429 mmol) and **(1)** (0.156 g, 0.429 mmol) in a molar ratio (1:1) (phosphine : complex) . The mixture was stirred for 1hour then refluxed for another 3 hours to afford a clear solution, The resulted solution was cooled at room temperature, filtered off and set aside to evaporate slowly. The white precipitate formed was filtered off, and dried under vacuum. (Yield: 0.173 g, 58%).

Synthesis of [Zn(dppp)(κ^1-2-mbm)(κ^1-2-mbn)] (5)

Ethanol (25 cm^3) was added to a mixed solid of dppp (0.117 g, 0.319 mmol) and **(1)** (0.132 g, 0.319 mmol) in a molar ratio (1:1) (phosphine : complex) . The mixture was stirred for 1hour then refluxed for 2 hours to afford a clear solution, which was filtered off and set aside to evaporate slowly. The resulting white gum formed washed with diethylether to afford white solid. The resulting solid was recrystallized from acetone to afford a yellowish white powder, which was filtered off and dried under vacuum at 50^{o}C (Yield: 0.186 g, 77%).

Synthesis of $[Zn(dppb)_2(\kappa^1$-2-mbm)(κ^1-2-mbn)] (6)

Ethanol (20 cm^3) was added to a mixed solid of dppb (0.165 g, 0.366 mmol) and **(1)** (0.067 g, 0.183 mmol) in a molar ratio (2:1) (phosphine : complex) . The mixture was stirred for 1hour then refluxed for 3 hours to afford a clear solution,. The solution was left to cool at room temperature, filtered off and set aside to evaporate slowly to afford a white powder containing crystals which was filtered off and dried under vacuum at 50^{o}C (Yield: 0.116 g, 82%).

Synthesis of $[Zn(dppf)_2(\kappa^1$-2-mbm)(κ^1-2-mbn)] (7)

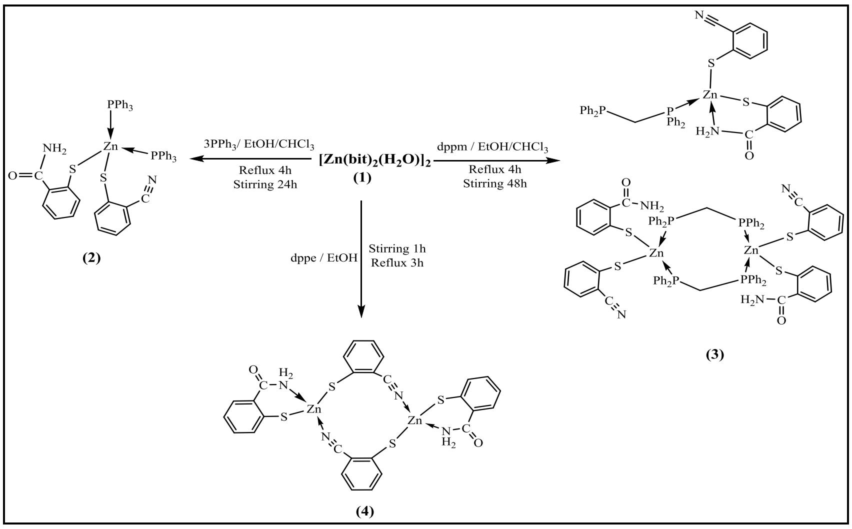
Ethanol (20 cm^3) was added to a mixed solid of dppf (0.197 g, 0.356 mmol) and **(1)** (0.065 g, 0.178 mmol) in a molar ratio (2:1) (phosphine : complex), an orange suspension was formed immediately after addition. The mixture was stirred for 1 hour then refluxed for 3 hours to afford a clear orange solution. The solution was cooled at room temperature, filtered off and set aside to evaporate slowly. The produced orange solid containing crystals was filtered off and dried under vacuum at 50°C recrystallized from hot acetone to afford an orange crystals (Yield: 0.126 g, 79%).

3. Results and Discussions

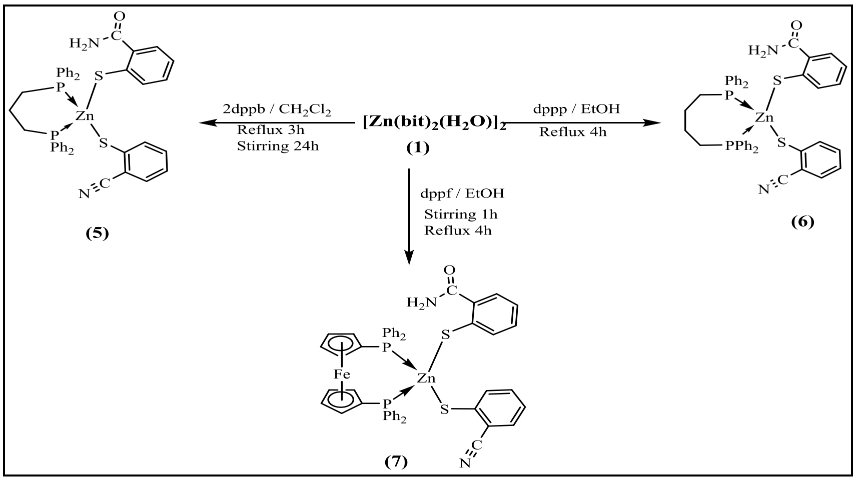
3.1 Synthesis of complexes 1-7

Addition of two equivalents of Na(bit) to zinc acetate $[Zn(OAc)_2].2H_2O$ in distilled water afforded the binuclear benzisothiozolinate bridged dimer $[Zn(bit)_2(H_2O)]_2$ (**1**) in 76% yields. Characterization data for this complex are given in Tables 1-3**.**

Treatment of (**1**) with two equivalents of the monodentate triphenylphosphine ligand Ph_3P afforded a single product characterized as $[Zn(PPh_3)_2(\kappa^1\text{-2-mbm})(\kappa^1\text{-2-mbn})]$ **(2)**. Reaction of (**1**) with the bidentate ligand, $Ph_2PCH_2PPh_2$ (dppm) afforded two complexes $[Zn(\kappa^1\text{-dppm})(\kappa^2\text{-2-mbm})(\kappa^1\text{-2-mbn})]$ **(3a)** and $[Zn(\mu\text{-dppm})(\kappa^1\text{-2-mbm})(\kappa^1\text{-2-mbn})]_2$ **(3b)**, while treatment of (**1**) with $Ph_2P(CH_2)_2PPh_2$ (dppe) afforded a single compound, charcteried as $[Zn(\kappa^2\text{-2-mbm})(\mu\text{-2-mbn})]$ **(4)**, unlike the other complexes the diphosphine ligand, dppe is not included in the product . Reactions of (**1**) with the (PPh_3,dppm,dppe) ligands (Scheme 1) Reaction of (**1**) with the bidentate ligands, $Ph_2P(CH_2)nPPh_2$, n = 3 (dppp), n = 4 (dppb), or $(CH_2)n = (C_5H_4)_2Fe$ (dppf) afforded complexes of the types $[Zn(dppp)(\kappa^1\text{-2-mbm})(\kappa^1\text{-2-mbn})]$ **(5)**, $[Zn(dppb)(\kappa^1\text{-2-mbm})(\kappa^1\text{-2-mbn})]$ **(6)** and $[Zn(dppf)(\kappa^1\text{-2-mbm})(\kappa^1\text{-2-mbn})]$ **(7)**, respectively (Scheme 2), characterization of the produced complexes are given later. In all the produced complexes the heterocyclic ring of the bit ligand has been broken from the nitrogen-sulfur bond and protonated from solvent to produce the 2-mercaptobenamide ligand (2-mbm) which in turn losses H_2O molecule to afford a 2-mrcaptobenonitrile ligand (2-mbn).



Scheme 1: Synthesis of complexes 2-4



Scheme 2: Synthesis of complexes 5-7

3.2 Characterization of complexes 1-7:

The prepared complexes are stable toward air and moisture, soluble in DMSO and DMF, and insoluble in distilled water, diethylether, ethanol, and methanol. The prepared complexes have been characterized by I.R. spectra, elemental analysis, conductivity measurements, ^{1}H nmr, and ^{31}P nmr spectra. Elemental analysis (Table 1) are in agreement with the suggested formula of the complexes. The molar conductance values of complexes measured in DMSO at room temperature (Table 1) are low suggesting that complexes **1-7** are non-electrolytes [16].

I.R. spectra of the prepared complexes (Fig **1-3**), and the selected I.R. values are given in Table 2). displayed the most noteworthy and unexpected spectroscopic feature; a strong absorption bands within 3180-3491 cm^{-1} range attributed to $\upsilon(NH_2)$, 2212-2218 cm^{-1} assigned to $\upsilon(C{\equiv}N)$ and 1643-1650 cm^{-1} range assigned to $\upsilon(C{=}O)$ [17-23]. These bands support the unexpected break down of the N-S bond of the benzisothiozolinate heterocyclic ring and the protonation to produce the 2-mbm ligand which then losses H_2O molecule to produce the 2-mbn ligand. The i.r. spectra of complexes **2,3** and **5-7** displayed bands within the 1429-1435 cm^{-1} and 507-540 cm^{-1} range attributed the υ(P-Ph) and υ(P-C) [24-26], indicating the presence of the phosphine ligands in the products. These bands were absent in the i.r. spectrum of complex **4**, indicating that the dppe ligand is not included in complex **4**.

The ^{31}P-{^{1}H} nmr spectra of the prepared complexes **2, 5, 6** and **7,** displayed a single peak each at δP = 29.27, 30.02, 32.86 and 36.27 ppm respectively, which indicates the presence of a single isomer each. The spectrum of **3** showed a singlet at δP = 31.44 ppm attributed to the complex containing a bridging dppm [27-30], [Zn(μ-dppm)(κ^1-2-mbm)(κ^1-2-mbn)]$_2$ **(3a),** the spectrum also showed two doublets at δP_A = -28.50 and δP_X = 28.05ppm with $^2J_{PP}$ = 87Hz, This clearly indicates that the two phosphorus atoms are non-equivalent, and attributed to uncoordinated and coordinated end of dppm respectively [27-30] in [Zn(κ^1-dppm)(κ^2-2-mbm)(κ^1-2-mbn)] **(3b)**.

The spectrum of the reaction product of dppe ligand with [Zn(Bit)$_2$(H$_2$O)]$_2$ (**1**) showed no ^{31}P nmr signal. It is clearly indicates that the product (complex **4**) does not contain phosphine in its structure.

The ^{1}H-NMR spectra of **2-7** complexes displayed the expected signals for the mbm and mbn ligands as well as the phosphines ligands (data are given in Table 3).

Conclusions

In this work we have prepared a new complex of the type [Zn(bit)$_2$(H$_2$O)]$_2$ from the reaction of zinc acetate and sodium benzisothiozolinate with (1:2) molar ratio. Reaction of dimeric complex (**1**) with triphenylphosphine or diphosphine affords [Zn(PPh$_3$)$_2$(κ^1-2-mbm)(κ^1-2-mbn)](**2**), [Zn(κ^1-dppm)(κ^2-2-mbm)(κ^1-2-mbn)](**3b**), [Zn(μ-dppm)(κ^1-2-mbm)(κ^1-2-mbn)]$_2$(**3a**),[Zn(κ^2-2-mbm)(μ-2-mbn)](**4**), [Zn(diphos)(κ^1-2-mbm)(κ^1-2-mbn)](**5-7**) (diphos: dppp, dppb and dppf) as a results. In all these reactions the N-S bond of the heterocyclic benzisothiozolinonate ring is broken and protonated to produce the 2-mercaptobenzamide ligand (2-mbm), then the product loses H_2O molecule to afford a 2-mercaptobenzonitrile (2-mbn) ligand. The geometry of the complexes (**2-7**) is a tetrahedral around the Zn(II) ion.

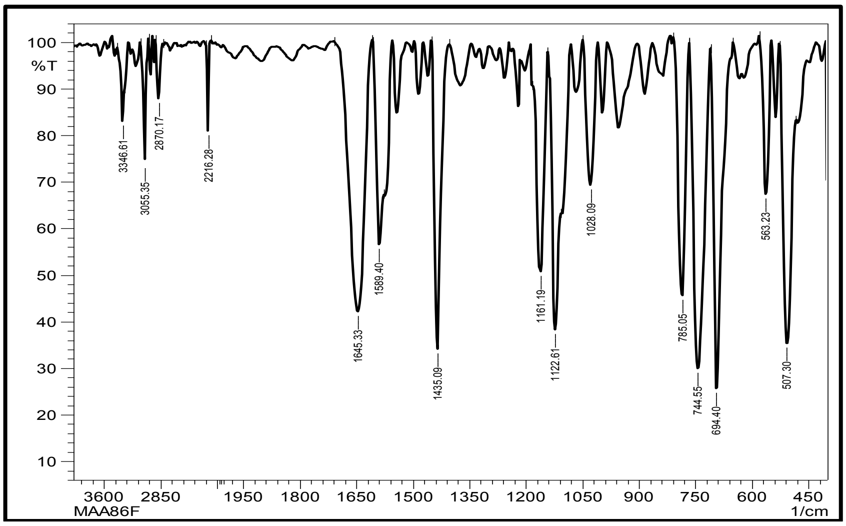


Fig. 1: IR spectrum of complexes 3a,b

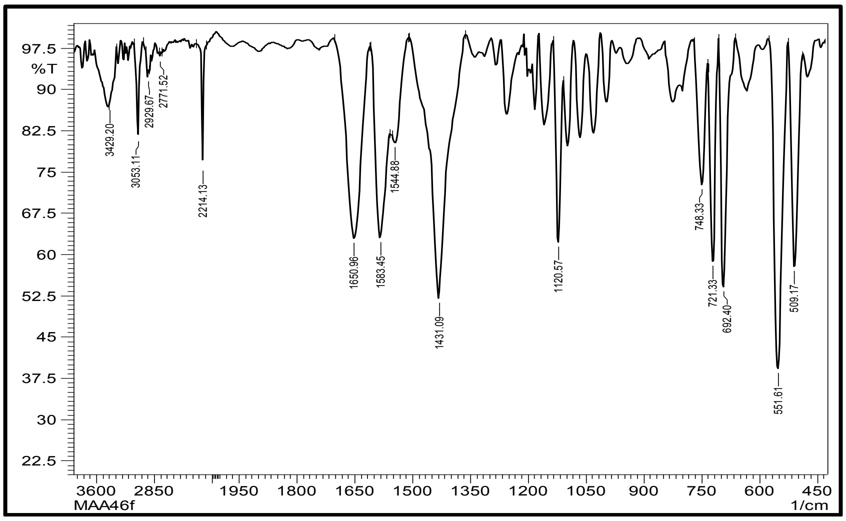


Fig. 2: IR spectrum of complex 5

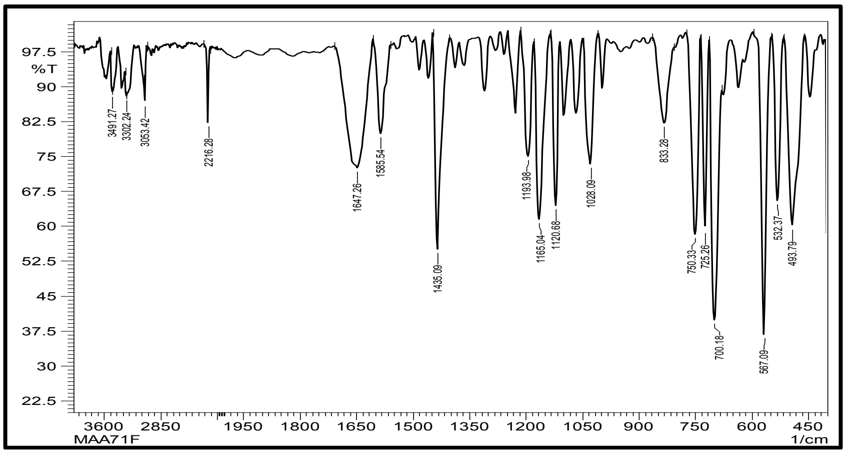


Fig. 3: IR spectrum of complex 7

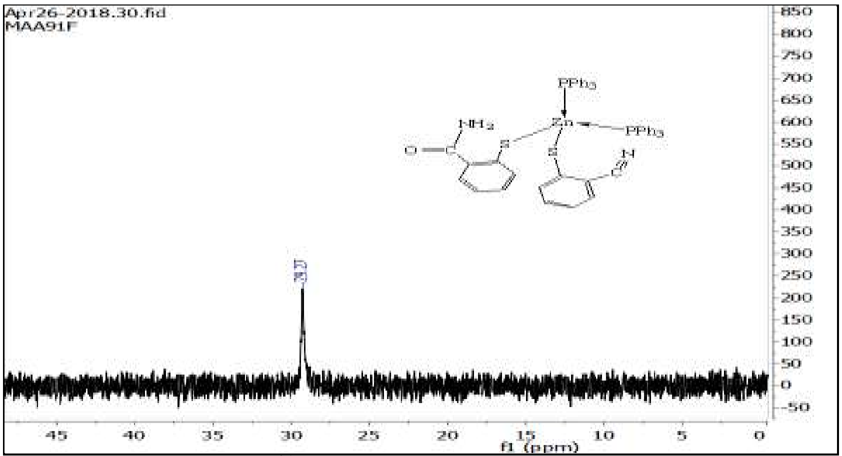


Fig. 4: ^{31}P NMR spectrum of complex 2

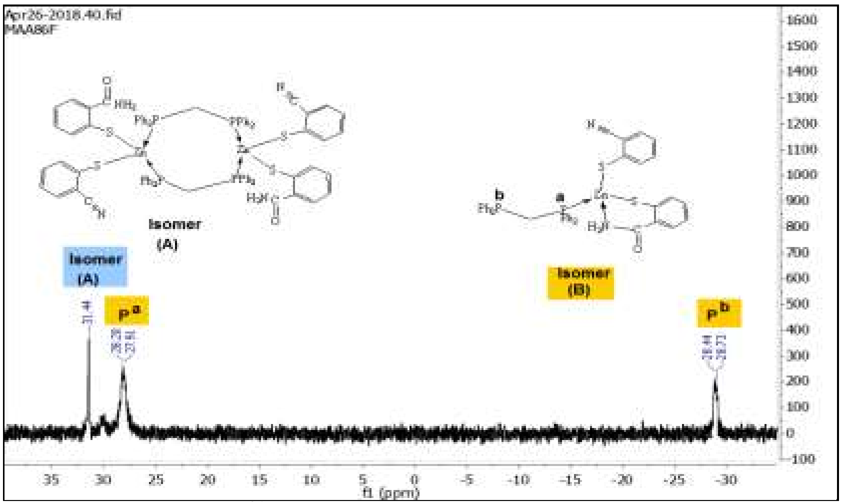


Fig. 5: ^{31}P NMR spectrum of complexes 3a,b

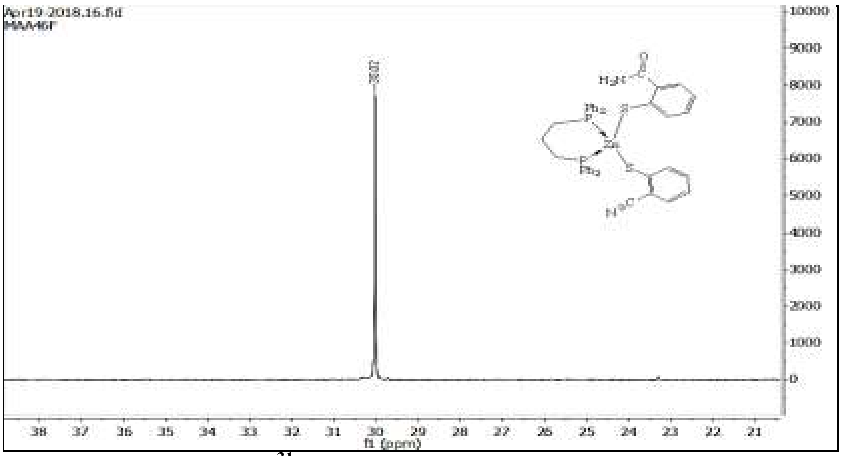


Fig. 6: ^{31}P NMR spectrum of complex 5

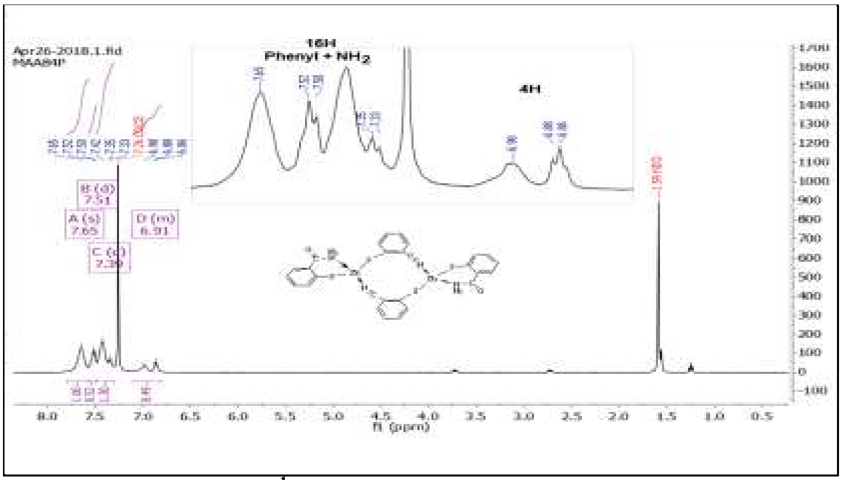


Fig. 7: ^{1}H NMR spectrum of complex 4

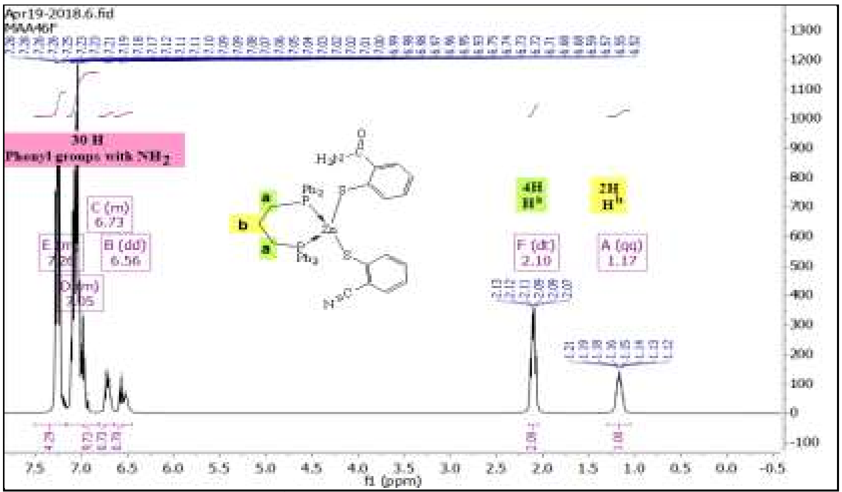


Fig. 8: ^{1}H NMR spectrum of complex 5

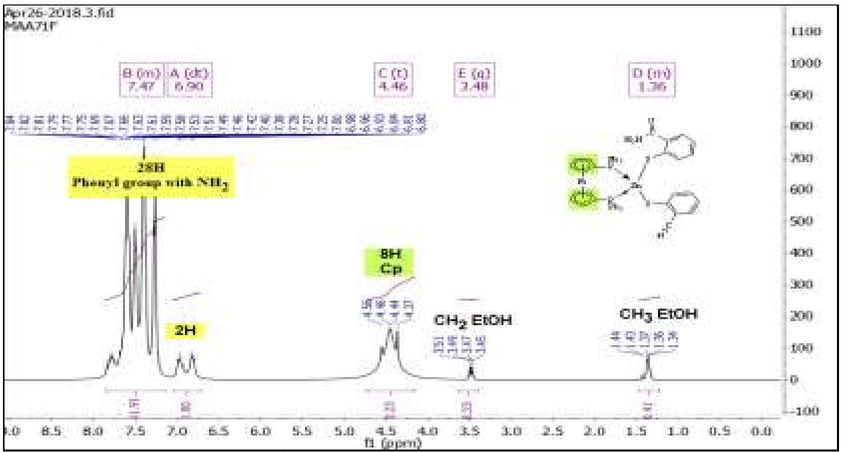


Fig. 9: ^{1}H NMR spectrum of complex 7

Table 1:Color, Yield, m.p, and elemental analysis of prepared complexes (1-7)

Seq.	Complexes	Yield (%)	m.p. (°C)	$\Lambda_M(\Omega^{-1}$ cm^{-2} mol^{-1}) 1×10^{-3}M DMSO	Elemental analysis Calc.(Found)%		
					C	H	N
1	$[Zn(bit)_2(H_2O)]_2$	76	320^a	4.6	46.05 (45.98)	2.16 (2.20)	7.53 (7.66)
2	$[Zn(PPh_3)_2(\kappa^1\text{-2-mbm})(\kappa^1\text{-2-mbn})]$	49	244D	3	68.50 (68.53)	4.64 (4.60)	3.21 (3.20)
3a **3b**	$[Zn(\mu\text{-dppm})(\kappa^1\text{-2-mbm})(\kappa^1\text{-2-mbn})]_2$ $[Zn(\kappa^1\text{-dppm})(\kappa^2\text{-2-mbm})(\kappa^1\text{-2-mbn})]$	41	115-117	3	------	------	------
4	$[Zn(\mu^2\text{-mbn})(2\text{-mbm})]_2$	58	187	7	49.54 (49.58)	3.03 (3.01)	5.91 (5.98)
5	$[Zn(dppp)(\kappa^1\text{-2-mbm})(\kappa^1\text{-2-mbn})]$	77	115	3	64.40 (64.44)	4.71 (4.75)	3.66 (3.67)
6	$[Zn(dppb)(\kappa^1\text{-2-mbm})(\kappa^1\text{-2-mbn})]$	82	165	3	64.88 (64.82)	4.88 (4.92)	3.63 (3.60)
7	$[Zn(dppf)(\kappa^1\text{-2-mbm})(\kappa^1\text{-2-mbn})]$	79	122-124	5	63.68 (63.77)	4.03 (4.01)	3.14 (3.10)

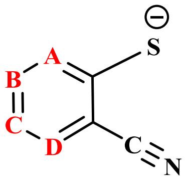
D= Decomposition ^{a}**=Does not melt up to 320 °C**

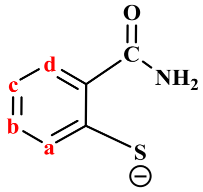
Table 2 : Selected IR stretching vibration bands (cm^{-1}) of the prepared complexes (1-7)

Seq.	Complex	υ (NH_2)	υ(C-H)		υ(C≡N)	υ(C=O)	υ(Ph-P)	υ(P-C)
			Ar.	Alph.				
1	$[Zn(bit)_2(H_2O)]_2$	------	3063w	------	------	1577s	------	------
2	$[Zn(PPh_3)_2(\kappa^1\text{-2-mbm})(\kappa^1\text{-2-mbn})]$	3180m 3354m	3053w	---------	2212m	1649s	1429m	540m
3a **3b**	$[Zn(\mu\text{-dppm})(\kappa^1\text{-2-mbm})(\kappa^1\text{-2-mbn})]_2$ $[Zn(\kappa^1\text{-dppm})(\kappa^2\text{-2-mbm})(\kappa^1\text{-2-mbn})]$	3346w	3055m	2870w	2216m	1645s	1435s	507s
4	$[Zn(\mu^2\text{-mbn})(2\text{-mbm})]_2$	3390w	3055w	---------	2218m	1643m	------	----------
5	$[Zn(dppp)(\kappa^1\text{-2-mbm})(\kappa^1\text{-2-mbn})]$	3429m	3053m	2929w	2214m	1650m	1431s	509m
6	$[Zn(dppb)(\kappa^1\text{-2-mbm})(\kappa^1\text{-2-mbn})]$	3315w 3377w	3053m	2929m 2858w	2216m	1647m	1431s	511s
7	$[Zn(dppf)(\kappa^1\text{-2-mbm})(\kappa^1\text{-2-mbn})]$	3302m 3491m	3053m	--------	2216m	1647m	1435s	532m

S= strong, m= medium, w= weak , b= broad , Ar.= Aromatic , Alph.=Aliphatic

Table 3 : ^{1}HNMR data, chemical shifts (δ ppm) and coupling constant (Hz) for the prepared complexes (1-7) measured in DMSO-d^6 or $CDCl_3$





Seq.	Complexes	δP (ppm)	δH* (ppm)
1	$[Zn(bit)_2(H_2O)]_2$	-------	7.88 (bs, 4H), 7.55 (bs, 2H), 7.37 (bs, 2H)
2	$[Zn(PPh_3)_2(\kappa^1\text{-2-mbm})(\kappa^1\text{-2-mbn})]$	29.27	7.48-4.28 (m, 40H)
3a **3b**	$[Zn(\mu\text{-dppm})(\kappa^1\text{-2-mbm})(\kappa^1\text{-2-mbn})]_2$ $[Zn(\kappa^1\text{-dppm})(\kappa^2\text{-2-mbm})(\kappa^1\text{-2-mbn})]$	(-28.58d; 28.05d) 31.44s	3.04 (t, 2H, $^3J_{HH}$=8Hz, CH_2-κ^1-dppm); 3.60 (t, 4H, $^3J_{HH}$=12Hz, CH_2-μ^2-dppm); 6.87 (td, 4H, H^a,H^d,H^A,H^D); 6.97 (s, 2H, H^1,H^4); 7.69-7.26 (m, 82H)
4	$[Zn(\mu^2\text{-mbn})(2\text{-mbm})]_2$	----	6.86 (t, 2H, $^3J_{HH}$=8Hz, H^b,H^c); 6.99 (bs, 2H, H^a,H^d); 7.65 (m, 16H)
5	$[Zn(dppp)(\kappa^1\text{-2-mbm})(\kappa^1\text{-2-mbn})]$	30.02	1.21-1.12 (m, 2H, CH_2^2-dppp); 2.13-2.07 (m, 4H, CH_2^1-dppp); 6.56 (dd, 1H, H^a); 6.75-6.68 (m, 1H, H^c); 7.28-6.93 (m, 28H)
6	$[Zn(dppb)(\kappa^1\text{-2-mbm})(\kappa^1\text{-2-mbn})]$	32.86	1.72-1.63 (m, 4H, CH_2^2-dppb); 2.26-2.19 (m, 4H, CH_2^1-dppb); 6.82-6.78 (m, 1H, Hb); 7.70-7.21 (m, 30H)
7	$[Zn(dppf)(\kappa^1\text{-2-mbm})(\kappa^1\text{-2-mbn})]$	36.27	4.56-4.37 (m, 8H, Cp-dppf); 6.81 (s, 1H, Ha); 6.98 (s, 1H, Hd); 7.84-7.25 (m, 28H)

References

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تفاعلات جديدة لكسر الاصرة N-S وفتح الحلقة بعد اضافة الفوسفينات الى معقد بنزايزوثايازولينون–خارصين (II)

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الملخص

يتفاعل مولين من ليكاند Nabit مع مول واحد من خلات الزنك في المحلول المائي ليعطي معقد من النوع $[Zn(Bit)_2(H_2O)]_2$ (1)، وعند معاملة المعقد **(1)** مع ثلاث مولات من ثلاثي فينل فوسفين ينتج معقد من النوع $[Zn(PPh_3)_2(\kappa^1\text{-2-mbm})(\kappa^1\text{-2-mbn})]$ **(2)**. حيث ان (2-mbm هـ 2–مركبتوبنزاميد و 2-mbn :2–مركبتوبنزونيترايل) اما عند معاملة **(1)** مع ليكاندات الفوسفين الثنائية $Ph_2P(CH_2)nPPh_2$ (diphos) (1 = n) (dppm) يُعطى معقدين $[Zn(\kappa^1\text{-dppm})(\kappa^2\text{-2-mbm})(\kappa^1\text{-2-mbn})]$ **(3a)** و $[Zn(\mu\text{-dppm})(\kappa^1\text{-2-mbm})(\kappa^1\text{-2-mbn})]_2$ **(3b)**، (2 = n) (dppe) اعطى معقد من النوع $[Zn(\kappa^2\text{-2-mbm})(\mu\text{-2-mbn})]$ **(4)**؛ و(3 = n) (dppp)، (4 = n) (dppe)، $(C_5H_4)_2Fe$) n = (dppf) ينتج معقدات من النوع $[Zn(diphos)\,(\kappa^1\text{-2-mbm})(\kappa^1\text{-2-mbn})]$ **(5–7)**، لقد اظهرت جميع المعقدات اعلاه ان الحلقة غير المتجانسة في ليكاند بنزايزوثايازولينون تعاني من كسر من جهة الاصرة N-S لتنتج ليكاند 2– مركبتوبنزاميد (2-mbn) او كسر الحلقة مع فقدان جزئية ماء لينتج ليكاند 2–مركبتوبنزونيترايل (2-mbm). شُخصت جميع المعقدات المحضرة بواسطة التحليل الدقيق للعناصر، مطيافية الاشعة تحت الحمراء، الموصلية المولارية، مطيافية الرنين النووي المغناطيسي للبروتون والفسفور.