Spectral Characterization of Polyvinyl Acetate and It's Modified Mercury Complex, Exploring It' S Structure and Applications

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Abstract

In this research work, a polymer metal complex was obtained by mixing aqueous solution with polyvinyl acetate at a certain ratio and temperature. The pure polyvinyl acetate and the synthesized polyvinyl acetate mercury complex was characterized with FT-IR, Uv, XRD and XRF spectroscopy. The FT- IR which confirms the presence of the important functional groups like the carbonyl at 1699.7cm⁻¹, the carbon to oxygen (C - O) at the 1060.9cm⁻¹, and so on, it also showed points to the coordination of the metal to the polymer. The Uv spectral shows that there was a transition shift form the lower energy to the Higher energy level which shows that the metal coordinated the polymer and a increased wavelength band which is as a result of conjugation of the polymer. The XRF shows that the elemental composition of the pure sample and the complex d sample which has higher amount of the mercury salt present at the polymer metal complex which indicated that the mercury coordinated to the polymer. The XRD shows the three sharp peaks at the polyvinyl acetate sample which indicates the crystalline structure of the polymer and when compared to the complex the XRD spectral data has a highest peak showing the coordination of polymer with the metal.

Keywords: polyvinyl acetate, mercury chloride complex, polymer, Characterization.

INTRODUCTION

Polyvinyl acetate (as known as PVA, PVAc, poly(ethenyl ethanoate), commonly known as wood glue, PVA glue, white glue, carpenter's glue, school glue, or Elmer's glue in the US, is a widely available adhesive used for porous materials like wood, paper, and cloth. Also an aliphatic rubbery synthetic polymer with the formula $(C_4H_6O_2)_n$, it belongs to the polyvinyl ester family, with the general formula -[RCOOCHCH₂]-. It is a type of Young et al, (1999). PVAc is a vinyl polymer that is prepared by the polymerization of vinyl acetate monomer (free-radical vinyl polymerization of the monomer vinyl acetate). Among many polymeric adhesives used in wood processing industry polyvinyl acetate has a rather wide application. It is used to glue tenon joints, doors, windows and other wooden articles. Bond strength is much higher than that of the wood itself Abu-saled, et al. (2012) However, polyvinyl acetate is nonresistant to moisture polymer and if such adhesive joints are exploited in moist environment its strength substantially decreases. This is caused by the hydrolysis of polyvinyl acetate present in adhesive joints when hydrophilic vinyl alcohol chains are formed in the macromolecule Gražulevičius, et al, (2023). Therefore, it is rather important to produce such a polyvinyl acetate (PVAc) dispersion which would make an adhesive joint sufficiently strong under moist conditions Abu-saled, et al. (2012). Polyvinyl Acetate is most widely used as an emulsion of PVAc polymers in water Amann, et al (2012). The emulsion is formed by polymerization in water of vinyl monomers, predominantly vinyl acetate, a process known as emulsion polymerization. The emulsion is white to off-white in color and is the familiar 'white glue' used in many household projects. Because of its resistance to attack by microorganisms and its low cost, this adhesive has replaced natural adhesives made from hide and casein in, for example, the manufacture of furniture. This adhesive sets by diffusion of the water into the wood and coalescence of the polymers. Setting times are comparatively rapid at room temperature. The set resins are light in color and often transparent, resulting in a glue line that is practically invisible. PVAc softens as its temperature is raised above room temperature, and it is less resistant to moisture and humidity than thermosetting resins. For this reason, PVAc adhesives are used in interior applications. In addition, PVAc tends to creep ('cold flow') under a sustained load. This limitation has been most serious when the adhesive is used to edgeglue lumber for solid stock, particularly high-density hardwoods. When such stock is exposed to low humidity, rapid moisture content changes through the end grain result in shrinkage stresses across the end of the bonded assembly. Often these stresses are of sufficient magnitude and duration to cause the adhesive to fail, resulting in open joints. Several modifications are used to enhance the resistance to moisture and to decrease creep of PVAc adhesive bonds Conner, (2017) One such method is the addition of other types of vinyl monomer during polymerization to improve the properties. A second method is to add cross-linking agents that increase the rigidity of the polymer. Because of the fact that PVAc is polymerized with minor amounts of vinyl alcohol, there are free hydroxyl groups on the polymer. Also, free hydroxyl groups can be formed by hydrolysis of the acetate groups. These hydroxyl groups offer sites for cross-linking. Cross-linking agents include strongly chelating metal salts such as chromium complexes. In addition, other adhesive resins such as UF, MF, and isocyanates have been used to advantage as chemical cross-linkers. Cross-linked PVAc are more rigid, have better moisture and heat resistance, and have greater initial tack Friedrich, et al. (2012). Metal complexes can play the role in a variety of applications, for instance, conversion of solar energy, polymeric light-emitting diodes, photo-refraction, chemical sensors, electrochromic as well as electro catalysis Gražulevičius, et al, (2023). Mercury (II) compounds are used in numerous expanses including polymers, cosmetics, paper, dyes, fluorescent lamps, and to a lesser extend in batteries.

2 MATERIALS AND METHODOLOGY

2.1 MATERIALS: Polyvinyl acetate (PVAc) molecular weight 190,000, mercuric chloride (Hg₃Cl), distilled water and ethanol was purchased from Onitsha head bridge market, Anambra state.

2.2 METHODOLOGY

2.2.1 SYNTHESIS OF POLYVINYL ACETATE

Wash and dry the apparatus for the synthesis. Measure out 10g of polyvinyl acetate and add to a 250 ml beaker, measure out 50ml of distilled water using the measuring cylinder and add the measured distilled water to the beaker that contains the polyvinyl acetate The resulting mixture was stirred using magnetic stirrer at 100° C temperature until all the polyvinyl acetate is dissolved. The solution is then filtered, washed with 150ml of ethanol and dried to form a powered solution.

2.2.2 SYNTHESIS OF MERCURY SALT

Wash and dry the apparatus for the synthesis. Measure out 2g of mercury salt and add to a 250 ml beaker, measure 20ml of distilled water and pour the measured ethanol into the beaker of the mercury salt and stir.

2.2.3 COMPLEX FORMATION

Measure out 20ml of dissolved polyvinyl acetate into a 250ml beaker, the 10ml of dissolved metal salt was poured into the beaker containing the polyvinyl acetate and Stir with magnetic stirrer for one hour at ambient temperature to form a homogenous mixture. The mixture was being filtered, washed with 150ml of ethanol and dried to have a powdered solution which is the complex.

2.2.4 CHARACTERIZATION

FTIR, UV-Vis spectroscopy, XRF, and XRD analyses were conducted to characterize the chemical structure and composition of the sorbents Connolly 2007. FTIR was used to identify surface functional groups relevant to oil sorption behavior (Okwuego, 2021 and Okwuego, 2023) Nkachukwu. *et al* 2025). UV-Vis spectroscopy provided insights into the electronic transitions and potential conjugated systems. XRF analysis determined the elemental composition (Mmuo *et al* 2024), while XRD revealed the crystalline phases present. These techniques collectively offered a comprehensive understanding of the sorbents' physicochemical properties influencing their sorption performance (Okwuego, 2022).

3.0 **RESULTS AND DISCUSSION**

Figure 1: FTIR Spectrum of the polyvinyl acetate Table 1. FTIR Spectrum of the polyvinyl acetate

Wavenumber (cm ⁻¹)	Peak Intensity	Functional Group	Vibrational Mode
3449.0	Medium	O–H (possible moisture)	O–H stretching
2948.3, 2855.0	Strong	-CH ₂ /-CH ₃ groups	Aliphatic C–H stretching
1739.9	Strong	Ester (-COO-)	C=O stretching (characteristic of PVAc)
1654.3	Medium	Possible C=C or adsorbed water	C=C stretching or H–O–H bending
1437.0, 1370.4	Medium	-CH ₂ /-CH ₃ groups	$\rm CH_2$ scissoring and $\rm CH_3$ bending
1237.5, 1020.6	Medium	Ester (-COO-)	C–O stretching
1103.3	Strong	Ester (-COO-)	C–O–C or C–O stretching
947.7, 842.6, 698.6	Medium	Vinyl group (C–H)	C-H out-of-plane bending



Figure 2: FTIR Spectrum of the polyvinyl acetate and mercury chloride

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Table 2: FITR Spectrum of the polyvinyl acetate and mercury chloride				
Wavenumber (cm ⁻¹)	Peak Intensity	Functional Group / Bond	Vibrational Mode / Notes	
3429.2	Broad	O–H stretching	Broad, likely from moisture or H- bonding	
2944.6, 2899.9	Strong	Aliphatic –CH2–	C–H stretching	
1736.3	Strong	Ester (C=O) group	C=O stretching (slightly shifted from pure PVAc)	
1669.7	Medium	Possibly due to coordination with Hg	Suggests Hg interaction with carbonyl or water	
1360.6, 1464.8	Medium	-CH ₃ bending	Methyl bending vibrations	
1244.6, 1080.9	Strong	C–O stretching (ester group)	Present in PVAc, slightly shifted, affected by HgCl ₂	
939.3, 827.5, 719.6	Medium	C–H out-of-plane bending	From vinyl backbone	
674.6	Medium	Possible Hg–Cl vibration	New band, likely due to mercury chloride presence	
2158.1	Weak	Possibly contaminant or overtone	Unusual for PVAc or HgCl ₂ , may be artifact	

All frequencies of the main characteristic bands of the polyvinyl acetate and its complex were presented in (Table 1 and Table 2), and the FTIR spectrum with their description and assignments are shown in (Figs. 1 and 2) respectively. In the FTIR spectra of polyvinyl acetate, a strong carbonyl stretching vibration transmittance peak (Vc=o) appears at 1699.7cm⁻¹, at 1103.3cm⁻¹ vibration transmittance peak of strong C-O-C stretching appeared, a strong transmittance peak at 2885.0cm⁻¹ is an alkane, caused by a C-H bending vibrations which shows that the molecule contains a -CH (Ochie et al 2025). The medium peak of band in 946.7cm⁻¹ region is a C=C bending vibration which indicates that vinyl acetate has been opened and polymerized to polyvinyl acetate. When PVAc is compared to PVAc-HgCl complex, the shape and position of the infrared spectrum transmittance peak of the complex is similar to that of PVAc. By comparing the two infrared spectra the carbonyl stretching vibration transmittance peak (v_0) is 1699.7 cm⁻¹, the transmittance peak of the complex did not show any shift in the wavenumber which indicate that there was no coordination in the carbonyl but the intensity changed from strong to a weak band. The transmittance peak of alkane moves to the higher wave direction from 2885.0cm⁻¹ to 2899.9cm⁻¹. The C-O-C vibration transmittance peak moved from 1103.3 to 1080.9cm⁻¹ which show that the lone pair electron of C-O-C coordinate with the transition metal ion (Okwuego et al 2025) and in addition, in the infrared spectra of the PVAc-mercury chloride at 857.3cm⁻¹ a typical medium stretching vibration peak appeared showing a present of an alkyl halides C-Cl and also at 1244.9cm⁻¹ a vibration band of alkyl had which indicates that the PVAc really coordinated to the transition metal to form a PVAcmercury chloride complex.



Figure 3: UV-Vis spectroscopy of polyvinyl acetate

Table 3: UV-Vis spectroscopy of polyvinyl acetateWavelength Range (nm) Absorbance Behavior Type of Transition Interpretation

~190– 210	Strong peak	absorpti	on π - π*	→ Indicates electronic	presenc transitio	e of ester on	-like groups	s; high	-energy
~230– 270	Gradual absorba	decre nce	ease	in Possibly (weak)	$n \rightarrow$	π* Weak absorb	transition; ance	less	intense
>280 Lit abs	tle t sorbance	o no	o _ No reg	significant	absorpti	on; confir	ms transpare	ency in	visible
Wavelen (nm) Figure U	A b gth 4: V	1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	2 2 7. 0 0						
spectros	copy of p	20 olyvinyl	acetate	30 and mercu	ry chlor	40) ide	0	50	00
-	1 V I				•				

Table 4.	UV spectroscopy of polyvinyl acetate and mercury chloride		
Component	Absorption Features	Contribution in Spectrum	
Polyvinyl Acetate	$\pi \rightarrow \pi^*$ around 190–210 nm (carbonyl group Weak $n \rightarrow \pi^*$ around 230–27 nm	m b) The strong peak < 210 nm and gradual 0 decrease up to ~ 270 nm align with this.	
Mercury Chloride (HgCl ₂)	Absorbs strongly below 25 due to charge transfer transitions May show some LMCT o transitions, especially in UV	0 nm (CT) Overlaps with PVAc in the <250 nm range. Sharp absorbance in this area may be d-d enhanced due to HgCl ₂ .	

The UV-vis spectrum in the table 3, fig. 3 and table 4, fig.4 respectively, shows the absorption pattern of pure PVAc and the PVAc modified with the mercury. The UV spectrum of polyvinyl acetate displayed an absorption of three different wavelengths with highest absorbance peak at 219nm which is the wavelength of maximum (λ_{max}). the polyvinyl acetate absorbed in the UV region at 219nm, 216nm, and 206nm, therefore the polyvinyl acetate does have any colour, it is colorless. When a light in the ultraviolet and visible region is absorbed by a material, it results in electron promotions from lower to the higher excited state in σ , π and n-orbitals, as stated in molecular orbital theory. Accordingly, $\sigma \rightarrow \sigma^*$, $n \rightarrow \pi^*$, $\pi \rightarrow \pi^*$ transitions will occur (Aziz *et* al., 2019; Sarma and Das, 2013). One of the most important factors affecting the wavelength of UV absorption by a molecule is the extent of conjugation. Molecular orbital calculations show that the energy difference between HOMO and LUMO decreases as the extent of conjugation increases (Mmuo et al 2024 and Libretext, 2023) also the wavelength that absorbs strongly corresponds to the energy difference between the HOMO and LUMO. Since the polyvinyl acetate has at 219nm which shows a shorter wavelength, therefore the polymer would have a higher energy transition. So, the λ_{max} of 219nm shows the present of H₂C=CH-CH=CH₂ which indicate that there is a long-chained polymer present, the wavelength peak at 206 indicates the presence of RCOO⁻R. Similarly, when compared to the polyvinyl acetate and mercury chloride UV spectra, it is observed that it only displayed one peak in the UV region just like the polyvinyl acetate spectra. The maximum absorption (0.0100) is found at λ_{max} 227nm, it is evident that the λ_{max} of polyvinyl acetate is shifted from 219nm to 227nm which shows that there was a coordination at the PVAc with the mercury chloride and the increase in the wavelength band is as a result of conjugation of the PVAc.

Sample Table of	PVAc
Chemical	Compostions
Components	(M)
SiO ₂	29.023
V ₂ O ₅	0.114
Cr ₂ O ₃	0.335
MnO	0.575
Fe ₂ O ₅	3.889
Co ₃ O ₄	0.116
NiO	0.087
CuO	1.275
Nb ₂ O ₃	0.102
MoO ₃	0.127
WO ₃	0.039
P_2O_5	3.323
SO ₃	2.636
CaO	9.010
MgO	4.727
K ₂ O	0.411
BaO	0.805
Al ₂ O ₃	27.188
Ta ₂ O ₅	0.000
TiO ₂	o.486
ZnO	1.122
Ag ₂ O	0.156
ClO	11.975
ZrO ₂	0.017
HgO	2.460
Element Table	of PVAc
Chemical	Compostions
Components	<u>(M)</u>
0	38.752
Mg	2.851
Al	14.390
Si	13.567
Р	1.450
S	1.056
Cl	11.975
K	0.341
Ca	6.439
Ti	0.292
V	0.064
Cr	0.229
Mn	0.446
Fe	2.720

Table 5: XRF of polyvinyl acetate sample table

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Ni	0.068
Cu	1.019
Zn	0.902
Zr	0.013
Nb	0.081
Mo	0.084
Ag	0.145
Ba	0.721
Та	0.000
W	0.031
Hg	2.279

Table 6: XRF of polyvinyl acetate and the mercury salt sample table

Sample Table PVAc/HgCl ₂		
Chemical	Compostions	
Components	(M)	
SiO ₂	2.098	
V ₂ O ₅	0.012	
Cr_2O_3	0.005	
MnO	0.019	
Fe ₂ O ₅	0.325	
Co ₃ O ₄	0.016	
NiO	0.000	
CuO	0.133	
Nb ₂ O ₃	0.062	
MoO ₃	0.079	
WO ₃	0.111	
P ₂ O ₅	0.000	
SO ₃	9.460	
CaO	2.011	
MgO	0.000	
K ₂ O	0.058	
BaO	0.000	
Al ₂ O ₃	1.663	
Ta ₂ O ₅	0.055	
TiO ₂	0.231	
ZnO	0.000	
Ag ₂ O	0.000	
ClO	17.409	
ZrO ₂	0.031	
HgO	66.224	

Element Table PVAc/HgCl ₂		
Chemical	Compostions	
Components	(M)	
0	13.359	
Mg	0.000	
Al	0.880	
Si	0.980	
Р	0.000	
S	3.789	
Cl	17.409	
К	0.048	
Са	1.437	
Ti	0.139	
V	0.007	
Cr	0.003	
Mn	0.015	
Fe	0.227	
Со	0.012	
Ni	0.000	
Cu	0.106	
Zn	0.000	
Zr	0.023	
Nb	0.049	
Mo	0.053	
Ag	0.000	
Ba	0.000	
Та	0.045	
W	0.088	
Hg	61.332	

The tables above show the X-ray fluorescence of pure polyvinyl acetate and polyvinyl acetate with mercury. The table 5 shows the XRF of the pure polyvinyl acetate sample and element table, that of 6 shows the modified polyvinyl acetate with mercury chloride sample and element table. The main focus of the XRF characterization is the mercury chloride attached to the polyvinyl acetate from the above table the result shows that there is present of mercury and chloride with the oxides of polyvinyl acetate containing ClO and HgO which accounted for about 11.975M and 2.460M respectively, some other oxides such as SiO₂, Cr₂O₃, Al₂O₃ and etc were also found to be present in small amounts. Then the oxides of the polyvinyl acetate modified with mercury chloride also contain ClO and HgO amounted to about 17.409M and 66.224M which shows that there is a sure present of the mercury salt attached to the polyvinyl acetate. The XRF results obtained from the ultimate elemental composition indicated a lot of

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elements present in the polyvinyl acetate and also with the mercury chloride modified polyvinyl acetate elemental composition the elements were present with mercury being the major element found followed by chlorine that is 61.332M and 17.409M, another element with high composition is oxygen which is 13.359M this has proven that the mercury is well attached to oxygen of the polyvinyl acetate. If the elemental composition is well studied it is noticed amount of the mercury increased in the table of polyvinyl acetate modified with mercury and the chlorine decreased in the table.



Figure 5: The XRD Spectrum of the Polyvinyl Acetate



Figure 6: The XRD Spectrum of Polyvinyl Acetate complex with mercury metal

The figure 5 and 6 shows the XRD of the polyvinyl acetate and polyvinyl acetate/mercury chloride respectively. The spectra data of the polyvinyl acetate sample shows three sharp peaks and this indicates the crystalline structure of the polyvinyl acetate but when compared to the complex form the spectra data exhibit three broad peaks at $2\theta = 14.88(9)$, 26.61(5), and

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40.89(11) reflecting the amorphous nature of the polyvinyl acetate/mercury chloride. Each of the 2 θ has a phase name, at 14.88(9) it is Terlinguaite: 2 0 0,Osumilite: 1, at 26.61(5), is known as Cinnabar, syn: 1 0 1,Osumilite and at 40.89(11) is said to be Terlinguaite: 0 0 4,Osumilite: 2. The 2 θ also has a chemical formula each, the 14.88(9) shows the formula as Hg² O Cl,K - Na – C, the 26.61(5) has its chemical formula as Hg S,K - Na – Ca and the 40.89(11) which is the highest peak shows the chemical formula of Hg²OCl which means that the polyvinyl acetate is well coordinated to the mercury chloride. The XRD spectra data of complex with the highest peak confirms the present confirms that the coordination of the polymer and the mercury chloride





4,1 APPLICATIONS OF THE POLYVINYL ACETATE MODIFY WITH THE MERCURY SALT.

The modification of polyvinyl acetate with a mercury was done to improve its physical properties can be applied in some aspect such as -;

High toughness -; the polyvinyl acetate is also known as PVA glue or white/wood glue, is widely recognized adhesive. While PVA glue offers some degree of water resistance, it is essential to understand its limitations when it comes to waterproofing. PVA glue excels in bonding porous materials such as wood, paper, and fabric. It forms a strong bond by penetrating the fibers of the substrate, creating a secure connection. However, when faced with a prolonged exposure to water or high humidity, the water resistance of PVA glue diminish. It may soften or lose its adhesive strength, potentially compromising the bonded surface. When modified with a mercury it will help to improve its bonding strength to last longer than the normal PVA. Fast curing and bonding time -; time is of essence in many PVAc application. It takes a lot of time for any PVAc to set or to be ready but with the modification with the drying and setting time reduced which will help to yield more results faster.

Rusting -; the PVAc acts as a binder in paints but due to the hydrolysis property of PVAc, when used on a metallic surface it slowly absorbs water which at a certain time still causes rusting which is the important used of the paint to the metal. But with mercury modified PVAc it helps reduce the absorption of water which will help prolong the shell life of the metal.

5. CONCLUSION

Based on the present studies it can be concluded that the modification of the polyvinyl acetate with the metal salt was successfully carried out. The spectral characterization of the polyvinyl acetate and the mercury modified polyvinyl acetate was conducted using FT - IR, Uv, XRD, and XRF which help to conclude that the metal was well coordinated to the polyvinyl acetate it showed the present of metal in the content of the modified polyvinyl acetate and also the higher energy transition of the polyvinyl acetate and modified polyvinyl acetate.

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