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Solubility and Fourier-Transform Infrared Spectra of Ascorbic and Pyruvic Acids with Some Metals

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Abstract

In this work, the preparation of complexes containing metallic elements such as Mn(II), Fe(II), Co(II), Cu(II) and Zn(II) with ascorbic acid and pyruvic acid as ligands is presented. The characteristics of these complexes were determined and analyzed by Fourier-transform infrared (FTIR) spectroscopy, UV-visible spectrophotometry, and solubility test in polar and non-polar solvents, in addition to the determination of melting points and conductivity.

Keywords: Metal complexes; Ascorbic acid; Pyruvic acid; Spectroscopic analysis

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1. Introduction

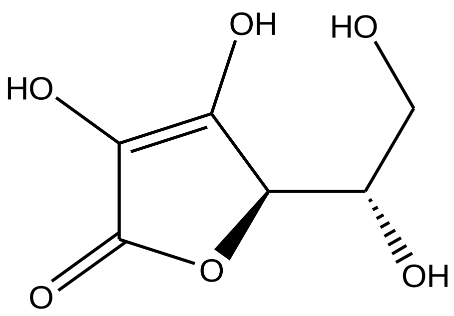
The solubility and Fourier-transform infrared (FTIR) spectra of ascorbic and pyruvic acids in combination with metals provide insights into their chemical behavior and interactions. Solubility studies reveal how these acids dissolve in various solvents when metals like calcium, magnesium, or zinc are present, forming metal-organic complexes. FTIR spectroscopy complements this by identifying specific functional groups involved in bonding. Characteristic peaks, such as shifts in hydroxyl or carbonyl stretches, indicate metal coordination. These findings are valuable for understanding their roles in biological systems, industrial applications, and nutritional science, particularly in supplement formulations or catalytic reactions involving metal-acid interactions.

Metal complexes or coordination complexes, is an atom or ion (usually metallic), bonded to a surrounding array of molecules or anions, which are in turn known as ligands or complexing agents Virtually all compounds containing metals consist of coordination complexes. Originally complex implied a reversible association of molecule, atoms or ions through such weak chemical bonds. As applied to coordination chemistry this meaning has evolved some metal complex are formed virtually irreversibly and many are bound together by bonds that are quiet strong [1-2].

Metal complexes with labile ligands have long been known to undergo ligand-substitution reactions with biomolecular targets. Metal ions can bind to nitrogen, sulfur or selenium atoms of the histidine cysteine, or selenocysteine residues in proteins leading to therapeutics effects [3].

The important metal present in the body is iron which plays a central role in all living cells. Generally iron complexes are used in the transport of oxygen in the blood and tissues. The heme group is metal complex, with iron as central metal atom, which bind or release molecular oxygen [4].

The structure of ascorbic acid has been widely studied [5] and was found to correspond to the enol of 3-keto-D-gulofuranolactone, it has a lactone structure with an endiol group.



L-ascorbic acid

Fig. (1) Structure of L-ascorbic acid

Table (1) Physical properties of ascorbic acid

Formula	Molar mass (g/mol)	Density (g/cm^3)	Melting point (°C)	Boiling point (°C)
$C_6H_8O_6$	176.12	1.694	190	553

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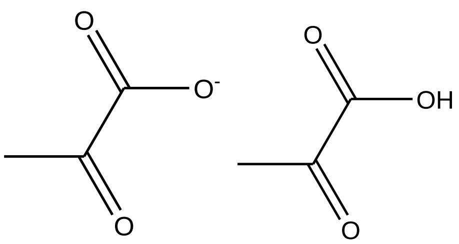
Biologically, L-ascorbic acid, are used to counteract scurvy. In pharmaceutics they are widely used [6,7] and fulfill the function of an antioxidizing agent in the food industry. Vitamin C, also known as L-ascorbic acid, is a vitamin found in food and used as a dietary supplement. As a supplement it is used to treat and prevent scurvy [8]. Evidence does not support use in the general population for the prevention of the common cold [9,10].

Vitamin C is a cofactor in at least eight enzymatic reactions, including several collagen synthesis reactions that, when dysfunctional, cause the most severe symptoms of scurvy [11]. In animals, these reactions are especially important in wound-healing and in preventing bleeding from capillaries. Ascorbate also acts as an antioxidant, protecting against oxidative stress [12].

Body requires vitamin C for normal physiological functions. It help in the metabolisms of tyrosine, folic acid and tryptophan [13]. It helps to lower blood cholesterol and contributes to the synthesis of the amino acid carnitine and catecholamine that regulate nervous system. It is needed for tissue growth and wound healing. It helps in the formation of neurotransmitters and increases the absorption of iron in the gut.

The chemistry of L-ascorbic acid and its derivatives includes various applications, biological [14,15] and industrial [16,17]. Major work and applications were done on L-ascorbic acid metal complexes and less attention was paid to metal complexes of alkylated derivatives of L-ascorbic acid [18-20].

Pyruvic acid ($CH_3COCOOH$) is the simplest of the alpha-keto acids, with a carboxylic acid and a ketone functional group [21]. Pyruvate, the conjugate base, CH_3COCOO^-, is a key intermediate in several metabolic pathways [22].



pyruvate pyruvic acid

Fig. (2) Structure of pyruvic acid and pyruvate

Pyruvic acid can be made from glucose through glycolysis, converted back to carbohydrates (such as glucose) via gluconeogenesis, or to fatty acids through a reaction with acetyl-CoA [23]. It can also be used to construct the amino acid alanine and can be converted into ethanol or lactic acid via fermentation. Metabolism of glucose known as glycolysis [24]. One molecule of glucose breaks down into two molecules of pyruvate.

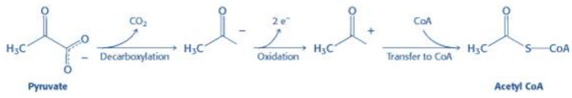


Fig. (3) Transformation of pyruvate to Acetyl CoA

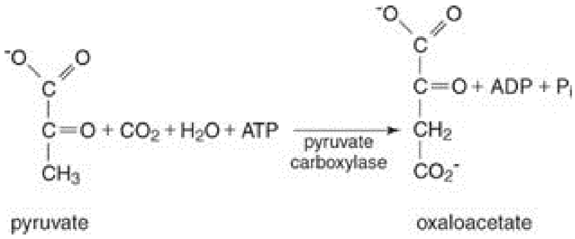


Fig. (4) Transformation of pyruvate to oxaloacetate

2. Experiment part

Chemicals are provided from different companies such as: Merck, Fluka, and Sigma-Aldrich. These chemicals are shown in table (2).

Table (2) Chemicals and its formula

Name	Molecular formula
Pyruvic acid	$C_3H_4O_3$
Ascorbic acid	$C_6H_8O_6$
Sodium hydroxide	NaOH
Copper chloride dihydrate	$CuCl_2.H_2O$
Zinc chloride	$ZnCl_2$
Manganese chloride tetrahydrate	$MnCl_2.4H_2O$
Cobalt chloride hexahydrate	$CoCl_2.6\ H_2O$
Ferrous sulfate heptahydrate	$FeSO_4.7\ H_2O$
Ethanol absolute	C_2H_5OH

The following instruments and apparatuses were used for tests and characterizations:

1- Balance (HR-200) .

2- Micropipette) 5-50 μL) & (5-1000 μL.

3- Fourier-Transform Infrared Spectra (FTIR) FT7600 Lambda.

4- Hotplate stirrer.

5- Electrothermal 9300 Engineering.

6- Shimadzu version 1.11 UV-1650 PC 2009.

7- Conductivity Meter Model Mi180 - MARTINI).

Complexes are prepared by reaction metal salt with ligands as ratio 1:1:1; m.mole of metal salt is dissolved in 10 ml of solvent, then it is added to 0.165 g of ascorbic acid in 10 ml solvent which it is added 2 mole from 0.104 g KOH in 10 ml solvent with stirring, then 0.11 g in 10 ml solvent is added to it. The mixture is stirring and heated by reflux in 80 °C for 3 hours, then cooling the mixture for 24 hours, filter, washing it by ethanol, drying in oven [25].

3. Results & Discussion

Melting points are measured for complexes by Electrothermal 9300 Engineering as shown in table (3). The results appeared high thermal stability for complexes. The measurement results of FTIR for ligands and complexes by FT 7600 Lambda with KBr disk in the spectral region 400-4000 cm^{-1} are shown in table (4).

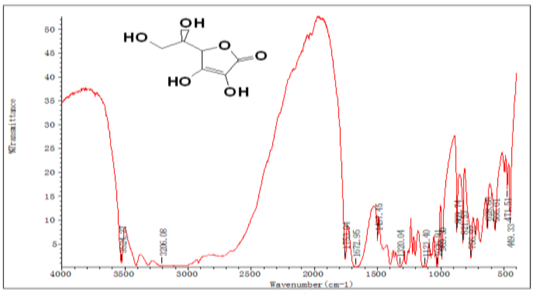


Fig. (5) FTIR spectrum for ascorbic acid

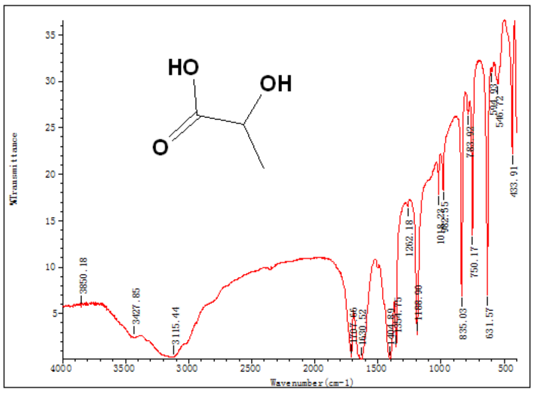


Fig. (6) FTIR spectrum for pyruvic acid

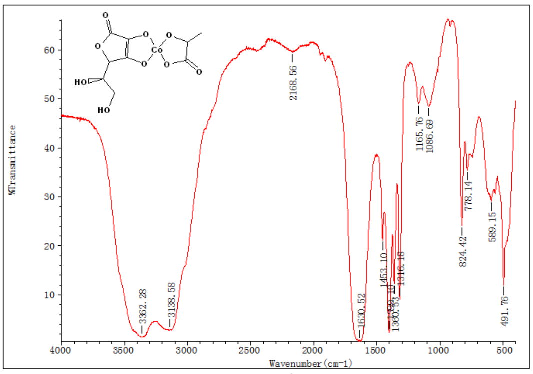


Fig. (7) FTIR spectrum for [Co(Asc.)(Pyr.)]

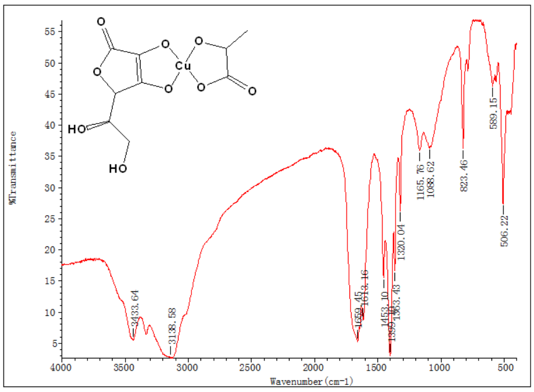


Fig. (8) FTIR spectrum for [Cu(Asc.)(Pyr.)]

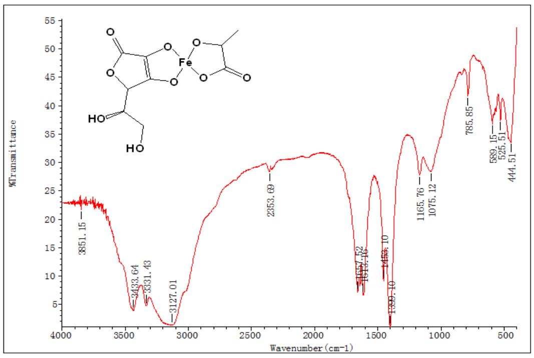


Fig. (9) FTIR spectrum for [Fe(Asc.)(Pyr.)]

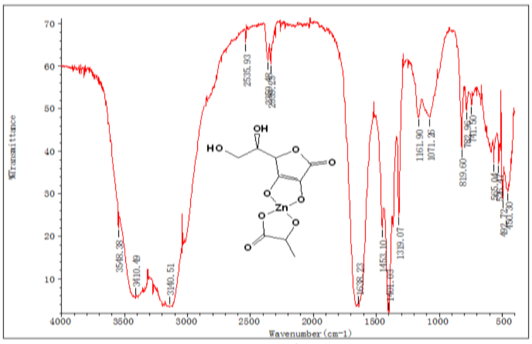


Fig. (10) FTIR spectrum for [Zn(Asc.)(Pyr.)]

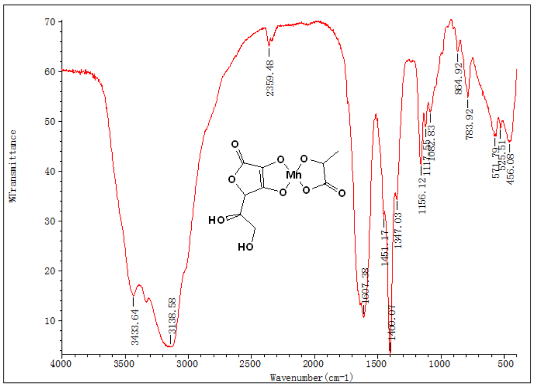


Figure (11) FTIR spectrum for [Mn(Asc.)(Pyr.)]

FTIR spectra for ascorbic acid and pyruvate appeared distinguished absorptions and identically with literary [26]. Strong and wide bands for hydroxyl group of ascorbic acid (3524, 3410, 3313, and 3206 cm^{-1}), some of these bands disappeared after forming complexes. The absorption band at 1754 cm^{-1} indicates the formation of C=O bond, while the absorption band at 1647 cm^{-1} indicates the formation of C=C bond.

Solubility is measured for ligands & complexes in laboratory temperature by some common solvents as shown in table (5).

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Table (3) Some physical properties for ligands & complexes

Compound	M.W g/mol	M. P. (°C)	Yield (%)	Color	Elemental Analysis C.H.N
Ascorbic Acid	176.12	190	-	White	C, 40.92; H, 4.58; O, 54.50
Sodium pyruvate	110.044	>300	-	White	C, 40.00; H, 6.71; O, 53.28
[Cu(Asc.)(Pyr.)]	325.71	>400	89.2	Greenish	C, 33.19; H, 3.09; Cu, 19.51; O, 44.21
[Co(Asc.)(Pyr.)]	321.10	>400	82.8	Purple	C, 33.66; H, 3.14; Co, 18.35; O, 44.84
[Mn(Asc.)(Pyr.)]	317.10	>400	54.3	Pink	C, 34.09; H, 3.18; Mn, 17.32; O, 45.41
[Zn(Asc.)(Pyr.)]	327.55	>400	47.7	White	C, 33.00; H, 3.08; O, 43.96; Zn, 19.96
[Fe(Asc.)(Pyr.)]	318.01	>400	76.9	Brown	C, 33.99; H, 3.17; Fe, 17.56; O, 45.28

Table (4) FTIR spectral data for ligands and prepared complexes

Compound	Functional group	*V* Cm^{-1}	Compound	Functional group	*V* Cm^{-1}
Ascorbic Acid	-C=O	1753	[Mn(Asc.)(Pyr.)]	-COO	1607
	-C=O	1672		-C=O	-
	-OH	3206		-OH	3433
	-OH	3524		-OH	3138
	2(OH)	3206 – 3524		M-O	456
[Co(Asc.)(Pyr.)]	-COO	1630	[Zn(Asc.)(Pyr.)]	-COO	1638
	-C=O	1630		-C=O	1753
	-OH	3138		-OH	3548
	-OH	3362		-OH	3411
	M-O	491		M-O	492
[Cu(Asc.)(Pyr.)]	-COO	1613	[Fe(Asc.)(Pyr.)]	-COO	1614
	-C=O	1659		-C=O	1658
	-OH	3138		-OH	3433
	-OH	3433		-OH	3127
	M-O	506		M-O	525

Table (5) Solubility for ligands & complexes

Compound	Methanol	Ethanol	Acetone	Chloroform	DMF	DMSO	H_2O
Ascorbic Acid	+	+	-----	-	+	+	+
Sodium Pyruvate	+	+	-----	-	+	+	+
[Cu(Asc.)(Pyr.)]	-----	+	-	-	+	+	+
[Co(Asc.)(Pyr.)]	-	-----	-	-	+	+	-----
[Mn(Asc.)(Pyr.)]	-----	+	-	-	+	+	+
[Zn(Asc.)(Pyr.)]	-----	+	-	-	+	+	+
[Fe(Asc.)(Pyr.)]	-----	-----	-	-	+	+	-----