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FTIR Spectroscopic Analysis on Human Hair

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ABSTRACT: The paper reports FTIR spectroscopic data on human hair. The IR spectrum reveals the constituents, proteins, lipids and carbohydrates. The main protein is keratin, present in large quantity where as carbohydrate ions and phosphate ions are relatively in small quantity. The study suggested that IR spectroscopy can be used for identification, analysis of amino acids and various ions present in the human hair.

KEYWORDS: FTIR, Hair, Keratin, Human Hair

I. INTRODUCTION

IR spectroscopy has been used to characterize and to identify compounds or the purity of a material. It has been applied in biology for studying the structure and conformation of molecules like proteins, nucleic acids and lipids. The advances made in instrumentation have paved the way for its utilization in the study of biomaterials with respect to structure of macromolecular components and their conformations within the tissue in most of the cases; infrared spectroscopy gives rapid qualitative and quantitative identification of organic and inorganic constituents and their combinations in mineralized biological tissues. It can also supplement other physical and chemical methods of analysis for the determinations of components present in the biomaterials.

II. RELATED WORK

FTIR is commonly used to identify compounds or the purity of a material. Infrared radiation in the range of 4000 to 400 cm^{-1} is used to irradiate a sample. Organic material absorbs and converts the energy to vibrations of the chemical bonds which join the atoms. The wavelengths at which the molecules absorb at depend on the masses of the atoms, the force constraints of the bonds, and the geometric of the atoms. Different species in the molecules vibrate and rotate producing bands at particular frequencies (measured in cm^{-1}). The absorption regions for different moieties are generally known, so a spectra produced can be compared to the known values to identify the material. For a general example, C-C, C-O, and C-N absorb between 1300-800 cm^{-1}, C=O, C=C, C=N and N=O absorb at 1900-1500 cm^{-1}, C≡C and C≡N absorb from 2300-2000 cm^{-1}, and C-H, O-H and N-H absorb at 3800-2700 cm^{-1}. The spectra produced are plotted either % transmittance (%T) or absorbance (A) verses wave numbers (cm^{-1}) or wavelength (µm) (Silverstein et al., 1981) [1]. Early research performed using infrared spectroscopy (IR) to analyze hair samples were conducted by Alter et al [2]. the oxidation of hair keratin with attenuated total reflection (ATR) IR was studied. The samples used for comparison were untreated hair and bleached hair (treated with H_2O_2). The differences in the IR spectra after bleaching the hair showed an appearance of new peaks at 1175 and 1040 cm^{-1}. These peaks were due to sulfonates which are formed by oxidation of cysteine. Cysteine dioxide peaks, due to oxidation of cysteine, were observed at 1220 and 1310 cm^{-1}, appeared and increased in size after successive bleaching.

IR research has been carried out by Signori et al [3]. Using an ATR diamond cell IR method. They also measured the concentration of oxidative damage of hair due to bleaching, when compared to untreated hair. Although the differences in spectral result were not discussed, the method of obtaining the data was described as an excellent tool for obtaining spectra of hair. Further discussion of IR methods for hair analysis by M`artin compared ATR using ZnS cells and diamond cells. The diamond cells gave the most reproducible result (Martin, 1999)[4]. Although the previous Methods have suggested reproducible results to analyze the oxidative damage in hair, IR still poses difficulty of obtaining

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information about the damage treatments cause to the inside of hair fibers because IR only penetrates the outer position of hair. Micro ATR FTIR, in combination with a focal plane array (FPA) detector, has also been used to study the cross-section of hair fiber (Chan et al., 2005)[5].

Other FTIR studies involving hair include analyzing the hydrogen bonds around hair protein to understand the mechanism of improving the durability of hair-setting with a certain treatment (Itou et al., 2006)[6], and also studying isolated melanin's from fair, red and dark hair (Bilinska et al., 1991)[7]. IR has also been used to study protein sources other than human hair, such as horse hair (Lyman et al., 2000)[8], plant cutin (Benitez et al, 2004), along with human skin, nails, and lipids (Gniadecka et al., 1998)[9]. A different role of IR in the area of hair care has utilized an IR light source to apply a polymer coating or film on hair fibres to act as a protective layer. The IR irradiation increases the polymer's molecular weight, giving better performance (Witteler et al., 2001; Morinaga et al., 2006)[11]. A comparison of our spectra to spectra obtained by other researchers showed basic similarities, as far as peaks, observed (Alter et al., 1968; Strassburger et al., 1985)[12].Mohammed Ehteshamuddin Aziz et al [13], studied the spectroscopic Analysis of Keratanised Tissue –The Hair.

III. MATERIALS & METHODS

Eight Scalp hair from each of 8individuals (8 females) were collected. These Eight hairs were taken from 8 different persons of minimum and maximum age of 0.3 year to 75 year respectively. For experimental analysis hair were properly cleaned to remove dust oil and greasy material. The sample is cut in to very small pieces and mixed with potassium bromide (KBr) and pressed in a stainless steel dye to produce thin KBr pellet. The spectrum of the sample was recorded in FTIR spectrometer (Shimadzu FTIR-8400s) in the range of 4000cm^{-1} to 400 cm^{-1}.

IV. RESULTS & DISCUSSION

Fig.1, 2, 3 and 4 show FTIR spectrum of Human Hair of ages 0.3year, 20year, 37year and 74 year respectively. This spectrum reveals a series of bands of different intensities. Table 1 presents the data on wave numbers and corresponding Transmittance (%) obtained from FTIR spectra along with characteristic vibrations of different functional groups.

In order to analysis the data, The FT-IR spectrum has been divided into five regions. Region I (4000 to 3200 cm^{-1}) concerned with water and carboxylic group in human hair. In this region the focus is on the revelation of the nature of hydrogen bonding and the carboxylic acids. In Region II (3200 to 1400 cm^{-1}) the bands for functional groups are observed. The functional groups are hydrogen stretching, stretching vibrations lipid acyl group, asymmetric stretching in lipids and proteins were confirmed and the β pleated structures conformation has been obtained.

Region III (1400 – 900 cm^{-1}) has significant importance in the context of biological minerals and their combinations. The spectra of hair indicates the presence of glucose, deformation of carbohydrates and the characteristics of phosphate ion, carbon ion and also of some functional groups concerned with protein – the Keratin. Region IV (900 – 800 cm^{-1}) gives the SO bond esters as well as deformation and out of plane bending vibrations of NO_2-, NO_3- and carbonate ions which can be used to get the un saturation of Hair. Region V (800 – 600 cm^{-1}) related to cis – double bond (=CH), N-H wagging, CO_2 absorption and SO^2_4 - ions andNH_2.

The dominating bands at 1636 cm-1 in Human hair (Figure 1, 2, 3 and 4) provides the β pleated structural conformations of proteins from Amide I components. The wave number 1532 cm-1 and 1529 cm^{-1} has been observed in Human hair respectively, which may be originated due to peak region of proteins. These are related to the stretching vibrations of C=C bonds and N-H bonds respectively. A band around 1241 cm-1 in Human Hair is due to the C-N stretch with N-H bending vibrations and Amide III band components of protein. The bands at 1176 cm^{-1}, 1174 cm^{-1}, 1044 cm-1, 1034 cm^{-1}, 921 cm^{-1} and 918 cm^{-1} for both species are related to stretching vibrations of C-O, COH and C-C ring vibrations in carbohydrates. These bands are believed to be more specific to glucose. The bands at 1241 cm^{-1} for Human Hair are originated from P-O anti symmetric stretch and from P = O asymmetric stretch and are related to calcium phosphate ions.

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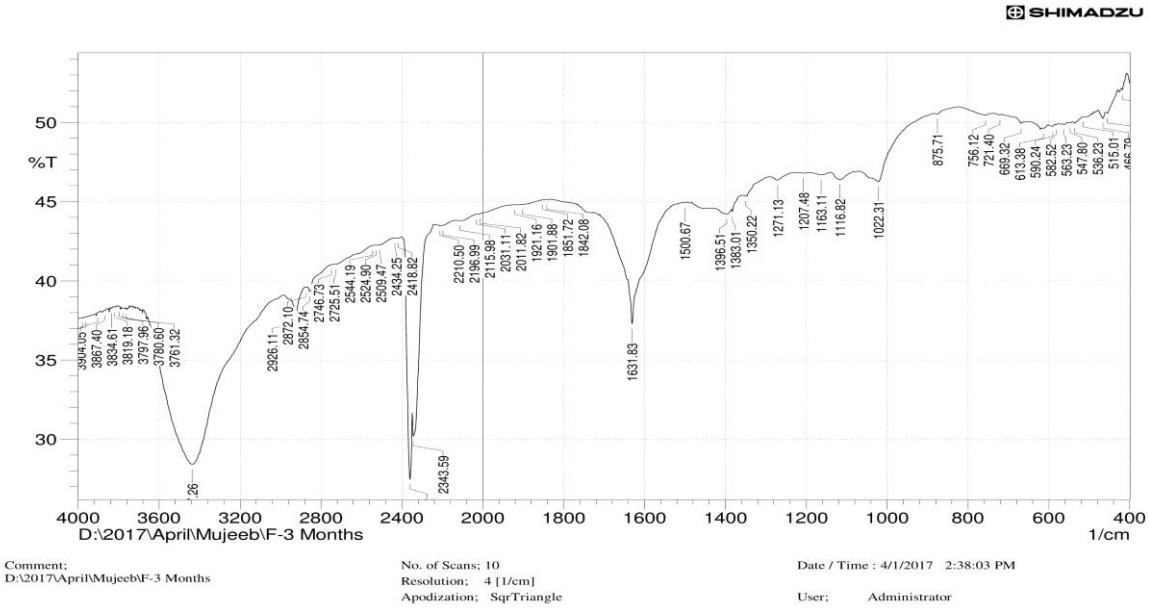
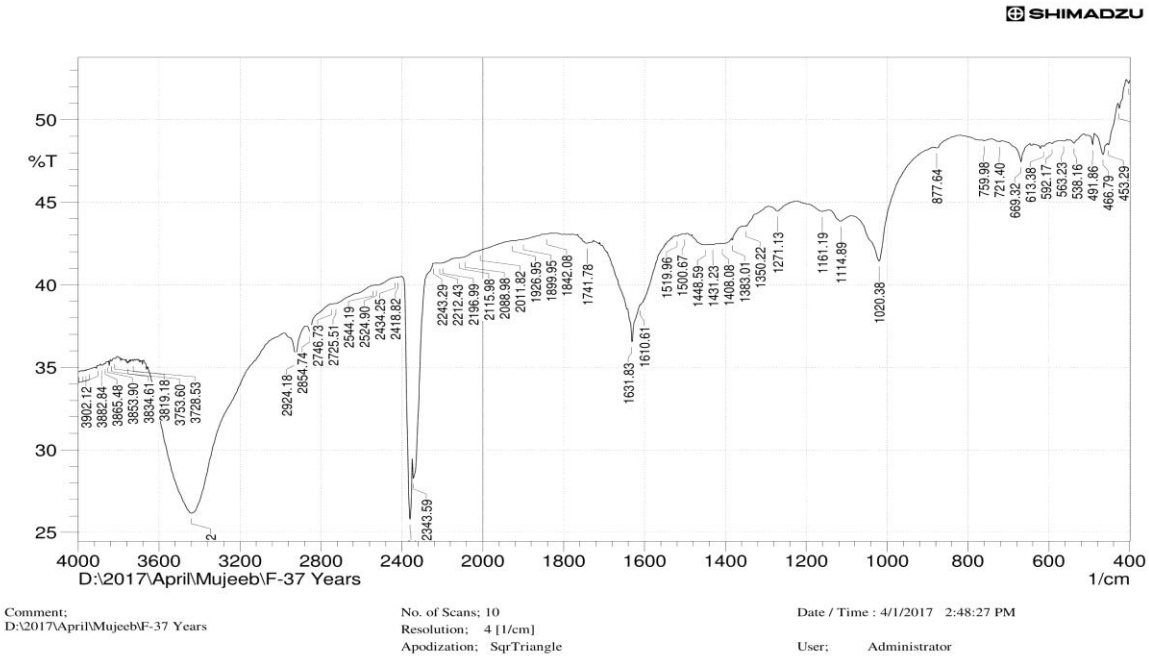


Wave Number (cm^{-1})

Fig. 1. FT IR spectra of Human Hair of age 0.3 year



Wave Number (cm^{-1})

Fig. 2. FT IR spectra of Human Hair of age 20year

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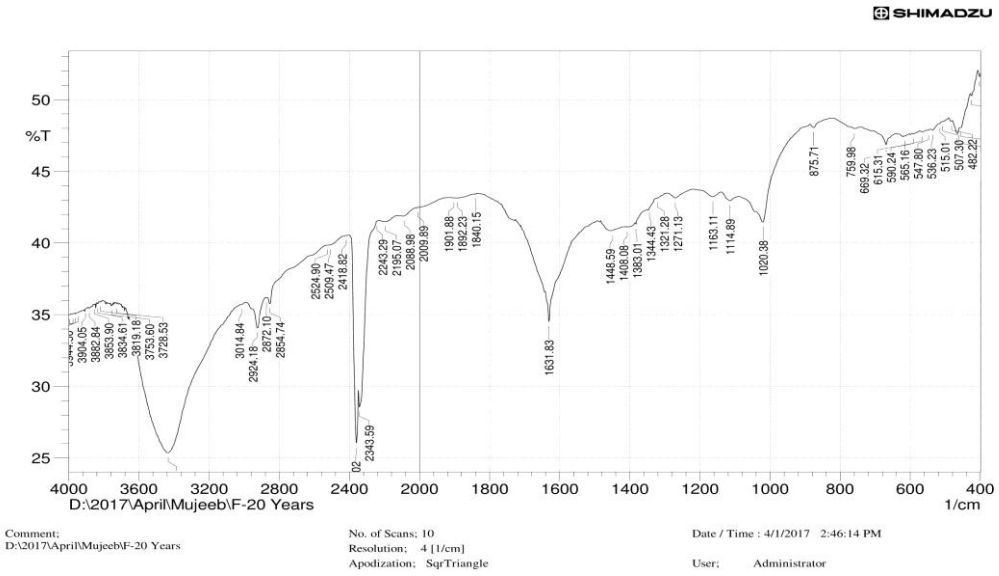
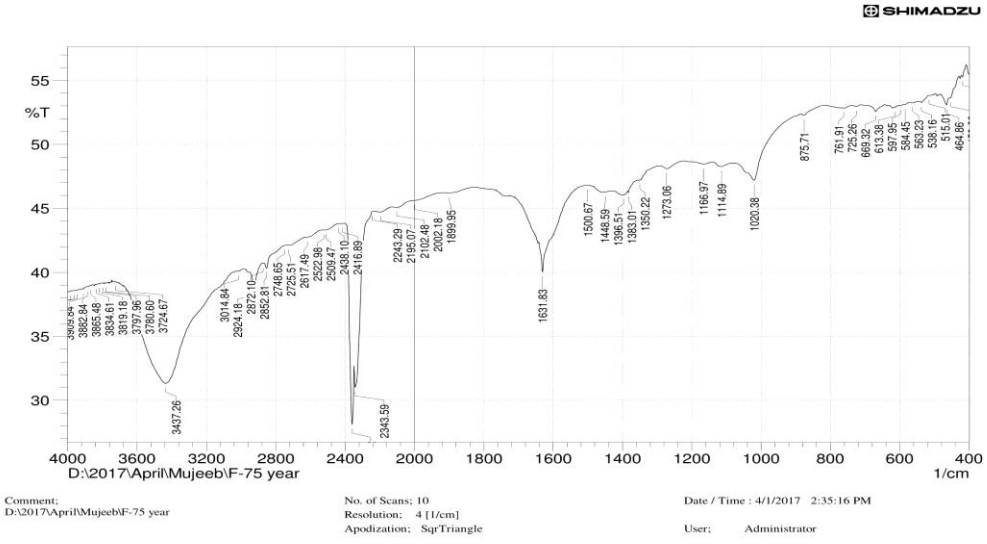


Wave Number (cm^{-1})

Fig. 3. FT IR spectra of Human Hair of age 37 year



Wave Number (cm^{-1})

Fig. 4. FT IR spectra of Human Hair of age 74 year

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Table1. FT IR data on Human Hair of Different ages

SNO	Wave number (Cm-1)	Transmittance %								Characteristics vibrations of functional groups
		0.3 yrs	6 yrs	10 yrs	20 yrs	37 yrs	45 yrs	52 yrs	75 yrs	
1	3837	38.25	41.61	34.085	35.766	35.388	19.125	30.122	39.031	H_2O (atmospheric absorption)
	3774	38.265							39.155	
	3740			34.092	35.622			30.087		
2	3292									O-H carboxylic acids and derivatives, alcohols and phenols
	3283									
	3072									C-H, CH_2, C=C alkenes
3	3068									Amide B, NH stretching
	2925	37.906	42.4	35.274	34.064	35.819		30.7280	38.906	C-H symmetric stretching of CH_2
	2858	39.320	43.280	36.2550	35.763	37.1700		31.636	40.329	C-H symmetric stretching of CH_2 in fatty acids, symmetric stretching vibrations of lipid acyl CH_2 groups
4	1639 1636	37.286	44.190	34.1930	34.517	36.5510	22.105	32.149	40.022	H-OH bending mode of water, NO2 bond in nitro compounds, Amide I band components β region pleated structures confirmation of proteins, C=C, C=N, (υC=C), NH_3 in υas and υs
	1532 1529		47.940							Amide II peak region – protein NH, (C-N), NO_2 bond in nitro compounds, carboxylic acids and derivatives
5	1455 1454		48.130		40.873	42.4130	24.910		46.277	CH_2, CH_3 asymmetric bending modes of lipids, proteins
	1241									Amide III band components of proteins (C-N), C-N stretching vibrations from amines from free amino acids.
	1238									P=O asymmetric stretching of PO - , phosphodiesters. 2
6	1176 1174	46.68	49.59	43.051	43.235		27.214		48.466	C-O, C-C, C-N, stretching C-O-H, C-O-C deformation of carbohydrates, DNA signals or maker bands
	1044						27.446			Carbohydrate bonds, suggests the C=O absorption of glycol protein
7	1034									C-O amide-I band, C-N, C-C, glucose
	921 918									C-O, C-C, C-N, stretching C-O-H, C-O-C deformation of carbohydrates, C-H and $=CH_2$

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	874	50.520	52.650	46.1900	48.059	48.2850	30.841	40.836	52.287	S-OR esters, out of plane bending, NO_2 -, NO_3 -, CO_2
8	**868** **828**		53.300			48.2850		41.248		
	827									
9	**756**	50.460	53.090	46.4780	47.980	48.7240		41.079	52.842	Cis-R, CH=CHR
	660	49.92	52.97	46.277	46.844	47.426	32.435	40.602	52.557	NH2 and N-H wagging, O-H bending In-plane, CO_2 (atmospheric absorption),
	643									C-H deformation, SO_4 2-, C-S in υ (C-S)

The study shows that the constituents of Human Hair are mainly Keratin which is in maximum quantity and glucose (relatively in small quantity). Carbonate ions and Phosphate ions are also present but in a very small quantity.

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