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INFRARED SPECTROSCOPY OF CHARGE TRANSFER COMPLEXES OF ELASTIN

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ABSTRACT

Elastin, a well-known stretchable two dimensional protein, is well-known among biomolecules. In the present study, elastin and its charge transfer complexes with organic acceptors such as TCNQ, TCNE, DDQ, chloranil and iodine have been studied using FTIR spectroscopy. Elastin is a weak donor. In the infrared spectra, it is observed that there is low-frequency hopping process revealed by square-power beta density. In CT complexes, gaussians are observed in mid-IR range. Elastin-iodine, elastin-DDQ and elastin-chloranil show range of nature of transition for the transition across a band gap.

Key words: *Elastin, Charge transfer complexes, Infrared spectra, Hopping process, Gaussian distribution, Nature of transition*

INTRODUCTION

Elastin, a two-dimensional stretchable protein [1], derives its name from elastic which has elasticity while stretching. Its unit is called desmosine [2] and is supposed to be a strong electron donor due to large number of COOH and NH_2 groups. Therefore, we study macromolecule like elastin here and its charge transfer complexes with organic acceptors. Elastin works as a weak donor.

EXPERIMENTAL DETAILS

Elastin is a white powder. First it was mixed with 1:1 molecular weight proportion with organic acceptors. Because elastin is a macromolecule its molecular weight is very high in amount because of very low molecular weights of acceptors, FTIR spectra did not show any change in the spectrum of elastin so elastin was again mixed with organic acceptors in equal volume proportions. This involved several-fold excess of acceptors. Acceptors selected were TCNQ(7,7,8,8,-tetracyano-p-quinodimethane), TCNE (tetracyano-p-ethylene), DDQ (2,3,-dichloro-5,6-dicyano-p-benzoquinone), chloranil(2,3,5,6-tetrachloro-p-benzoquinone) and iodine. These acceptors when large in amount reacted to form CT complexes with elastin. The CT complexes of elastin were taken in small amount (about 5%) and mixed with dry spectrograde KBr powder which was 95%. The mixtures were grinded till 5% of CT complex homogeneously dispersed into KBr powder. Circular discs were prepared using a die and a manually operated compressing machine. Discs were placed in dark chamber of GXFTIR single beam spectrophotometer of Perkin Elmer Company, USA.

The spectra in the range 400-4000cm^{-1} were recorded using a GXFTIR single beam spectrophotometer manufactured by Perkin Elmer company, USA, having resolution of 0.15 cm^{-1} a scan-range of 15,000-30 cm^{-1}, scan time 20 $scans^{-1}$, an optical phase detector(OPD) velocity of 0.20cms^{-1} and MIRTGS and FIRTGS detectors. A beam splitter of the opt KBr type was used having a range of 7800-370cm^{-1}. The spectra were recorded in purge mode.

RESULTS AND DISCUSSION

The FTIR spectrum of elastin is shown in Fig. 1a.

The material is transmitting in the range of 1800cm^{-1} to 2800 cm^{-1}. Thus it shows that the band gap of elastin is very large and does not have band gap in IR range. Elastin is an insulator. Between 1000 cm^{-1} and 1800 cm^{-1} there are large number of vibrational bands of elastin molecule and this range does not contain any well-defined background absorption [3] or electronic absorption envelope. However, in the low-frequency range below 900 cm^{-1}, a square-power beta density is seen in absorption profile. This beta density indicated a low frequency hopping process present in elastin. Either a carrier hops or it does not hop. This is a Bernoulli trial of probability theory. Bernoulli trial leads to a beta density as a probability distribution function. Half-power beta density arises in a neutral compound while square-power beta density arises in a dipolar compound which is polarizable when it is stretched. The square-power beta density [4, 5] is given by $\alpha = \alpha_0 K^{\alpha}(1-K^{\alpha})^{\alpha}$ where $K^{\alpha} = \frac{K-a}{b}$ and in this 'a' is initial point of the peak and 'b' is base width. This function has been fitted (Fig. 1b).

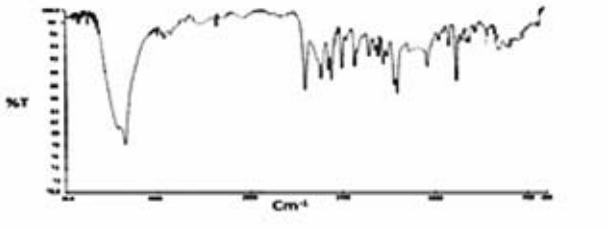

Fig. 1a: The FTIR spectrum of elastin.

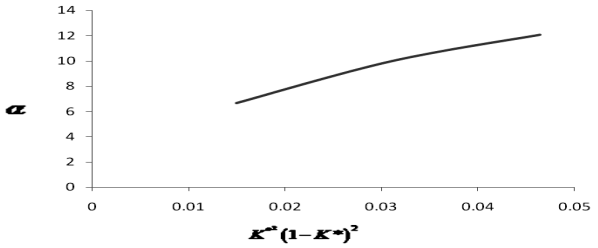

Fig. 1b: The square power beta density in elastin.

The FTIR spectrum of elastin-TCNQ is also shown in Fig. 2a.

The CT complex remains transmitting in the range 1800cm^{-1} to 3000 cm^{-1} and does not show development of any absorption. This indicates that elastin-TCNQ also does not contain any absorption due to transition across the band gap in IR range. Thus elastin-TCNQ also is a wide-band-gap semiconductor. However, the IR spectrum contains two

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gaussian background profiles –one in mid-IR range around 1500 cm^{-1} and one in low-frequency range around 700 cm^{-1}.

The gaussian bands are given by $\alpha = \alpha_0 \exp\left(-\frac{(k-k_0)^2}{2m_2}\right)$ where α_0 the maximum absorbption, is central wave number k and m_2 is the second moment of the distribution. This function is fitted by plotting $\ln\alpha \text{ vs } (k-k_0)^2$. Both the gaussian profiles are fitted (Fig. 2b).

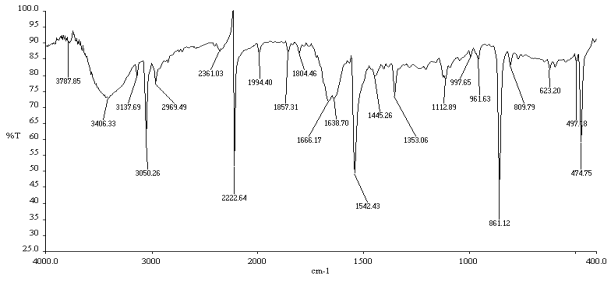

Fig. 2a: The FTIR spectrum of elastin-TCNQ.

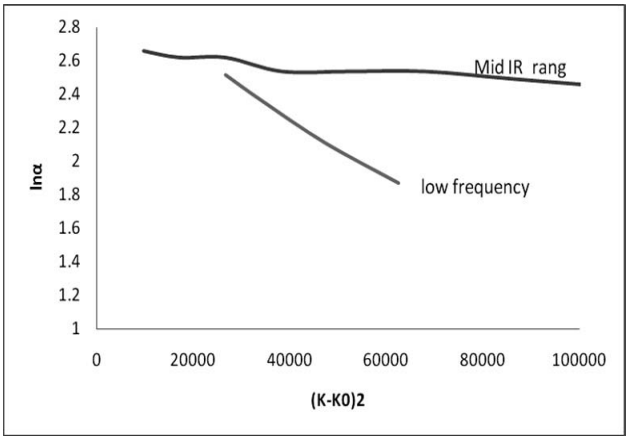

Fig. 2b: Mid-IR and low frequency Gaussian band in Elastin-TCNQ

The square-power beta density becomes gaussian distribution in the low-frequency region. This shows the charge carriers like polarons show band motion leading to gaussian distribution rather than a hopping process. This is the change incurred by TCNQ which stretches the bonds of elastin and polarons, rather than hopping among various sites of elastin, shows continuous motion. This mid-IR gaussian band shows similar band motion of polarons but in high frequency range. The results should be compared with α-keratin and it's CTCs with organic acceptors. α keratin is a fibrous protein and its CTCs show half-power beta density due to constrained motion of carriers across the linear chain fibre. Here the lattice vibrations have two degrees of motion in elastin and its CTCs. The gaussian distribution results due to dispersion of vibration in two-dimensions in planar elastin.

The FTIR spectrum of elastin-TCNE is shown in Fig. 3a.

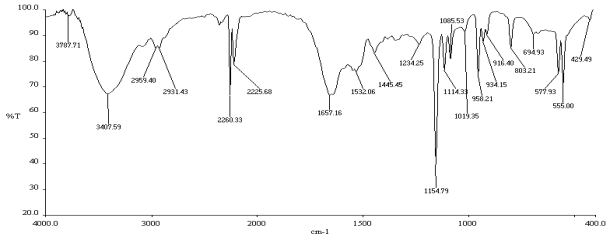

Fig. 3a: The FTIR spectrum of elastin-TCNE.

The spectrum is many respects similar to elastin-TCNQ spectrum. Again a transmitting range followed by two gaussian bands in background absorption at lower frequencies is observed. The two gaussian bands are tracked due to dispersion of polarons or a complex phonon in two-dimensions due to the force arising from TCNE molecules. The gaussian curves are fitted (Fig. 3b).

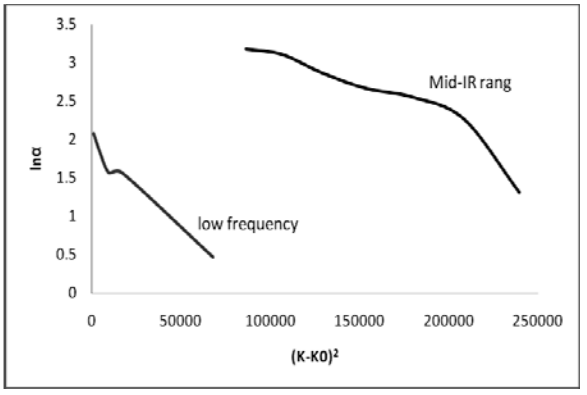

Fig. 3b: Mid-IR and low frequency gaussian band in Elastin-TCNE.

The FTIR spectrum of elastin-iodine is shown in Fig. 4a.

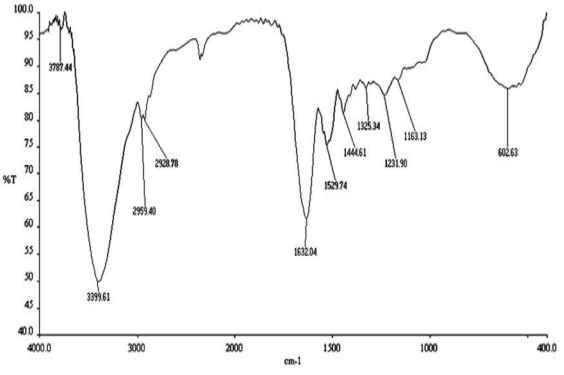

Fig. 4a: The FTIR spectrum of elastin-iodine.

This spectrum shows a range in which absorption develops in infrared range between 1800cm^{-1} and 3000 cm^{-1}. Thus the charge transfer interactions are strong enough to bring down band gap value to IR range. Thus halogens interact strongly with elastin. The mid-IR range between 1000 cm^{-1} and 1700 cm^{-1} shows a triangular type background absorption arising from imperfect nesting. The nature of transition is analyzed from Fig. 4b.

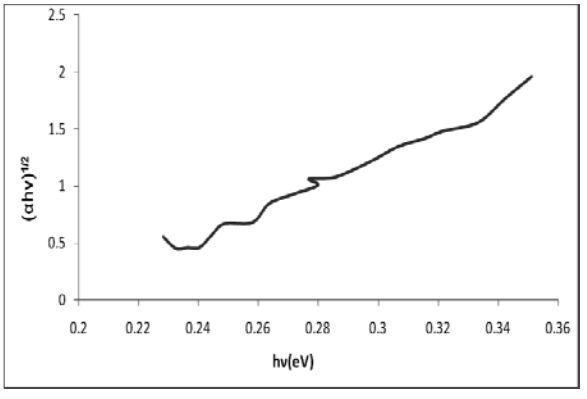

Fig. 4b: Nature of transition of elastin-iodine.

The low-frequency gaussian distribution around 600 cm^{-1} is also fitted which shown in Fig. 4c.

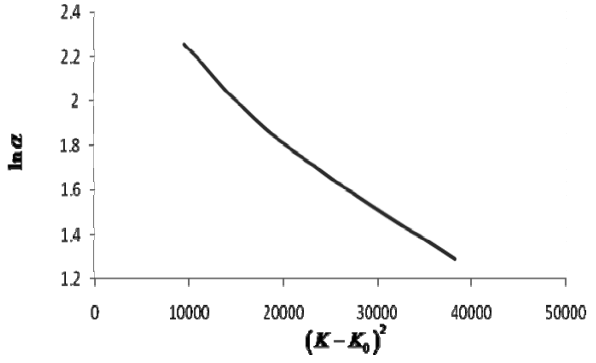

Fig. 4c: Low frequency Gaussian band in elastin-iodine.

The FTIR spectrum of elastin-DDQ is shown in Fig. 5a.

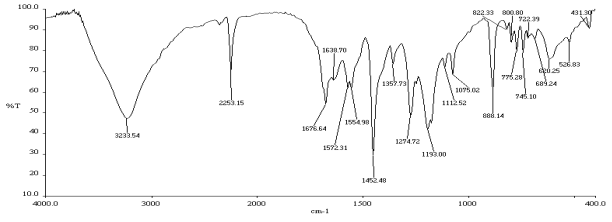

Fig. 5a: The FTIR spectrum of elastin-DDQ.

There exists a range (1800-2900cm^{-1}) in which absorption due to transition across band gap develops (Fig. 5b).

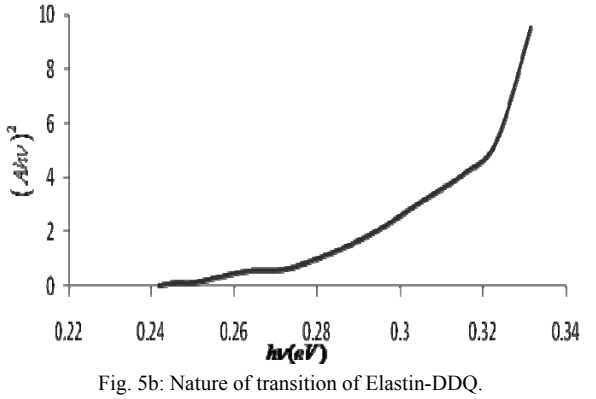

Fig. 5b: Nature of transition of Elastin-DDQ.

A pronounced gaussian band is observed in the mid-IR range. This gaussian distribution is fitted as shown in Fig. 5c.

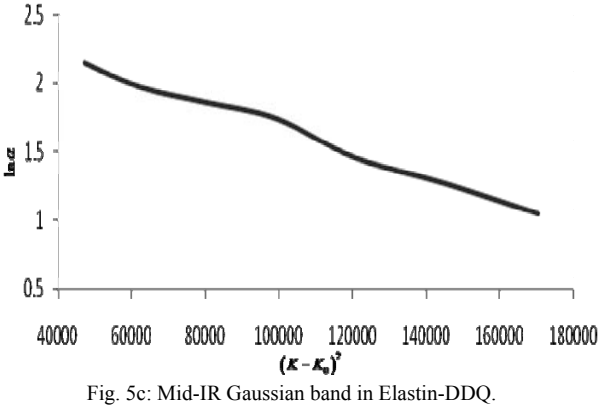

Fig. 5c: Mid-IR Gaussian band in Elastin-DDQ.

Finally, in low frequency range a Lorentzian or oscillator model is observed rather than a gaussian band or beta density. This shows presence of strong electron-phonon resonance in low-frequency range around 620cm^{-1}.

The FTIR spectrum of elastin-chloranil is found to be different which shown in Fig. 6a.

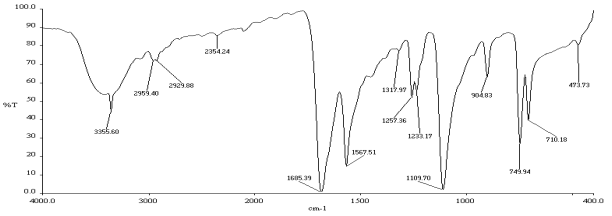

Fig. 6a: The FTIR spectrum of elastin-chloranil.

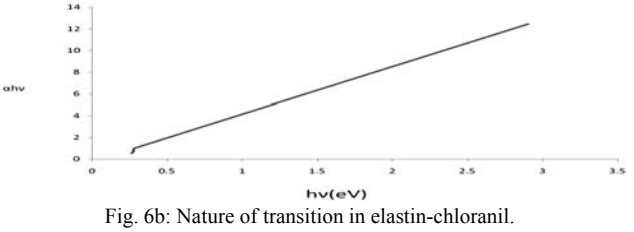

Fig. 6b: Nature of transition in elastin-chloranil.

Here apart from absorption of light due to transition across a band gap (Fig. 6b), a large number of repeated structures are observed. These structures can be ascribed to the oscillations in the density of states. Square-root singularity describes the shapes of these structures as found in one-dimensional systems of lattice vibrations. Such oscillations are found in magnetic field and here they seem to arise from transverse optical phonons. Thus elastin-chloranil can be used as molecular multivibrator.

The parameters of the gaussian distributions observed into CT complexes of elastin are summarized in table 1. The values of band gaps and nature of transitions are summarized in table 2.

Table - 1 The parameters of gaussian distributions observed in charge transfer complexes of elastin.

Name of complex	Mid-IR gaussian distribution			Low-frequency gaussian distribution		
	α_{max}	K_0	FWHM	α_{max}	K_0	FWHM
Elastin-TCNQ	85	1335.95	956.52	86.11	630	610.86
Elastin-TCNE	88.125	1467.3	597.89	93.125	608.69	310
Elastin-Iodine	-	-	-	86.36	606.38	329.79
Elastin-DDQ	85.714	1423.91	663.05	-	-	-

Table 2: Values of band gaps and nature of transition in CT complexes of elastin.

Name of the complex	Absorption function	Value the band gap (eV)
Elastin-iodine	$\alpha h\nu=A(h\nu-Eg\pm Ep)^2$ Allowed indirect transition	0.2
Elastin-DDQ	$\alpha h\nu=A(h\nu-Eg)^{1/2}$ Direct allowed transition	0.26
Elastin-chloranil	$\alpha h\nu=A(h\nu-Eg)$ Direct allowed transition	0.25

CONCLUSION

Elastin does form complexes with organic acceptors when the later are taken in large amount. Charge transfer interactions are strong and are sufficient enough to bring down band gap values to IR range in particularly with halogen like iodine and halogen-containing acceptors like DDQ and chloranil. This shows elastin interacts with chlorine atoms in DDQ and chloranil. The interaction is strongest in chloranil leading to the oscillations in the density of states of charge carriers.

REFERENCES

[1] Albert L. Lehninger (1987), *Principles of Biochemistry*: CBC Publishers & Distributors, Chpt. 6,pp. 123.

[2] Roger Baurain, Jean-Franqm Larochelle, and Franqois Lamy (1976), Photolysis of Desmosine and Isodensmosine by Ultraviolet Light, *Eur. J. Biochem*, 67: 155-164.

[3] Jacques I. Pankov (1971) *Optical process in semiconductor* , Prentice-Hall, Englewood Cliffs, NJ, pp. 34.

[4] Grubbs, Frank E. (1962) Attempts to Validate Certain PERT Statistics or 'Picking on PERT'. *Operations Research* **10(6)**, pp. 912-915.

[5] Keefer, Donald L. and Verdini, William A. (1993). Better Estimation of PERT Activity Time Parameters. *Management Science* **39(9),** pp. 1986-1091.

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Books

[16] Stebbins, G. L. (1974) *Flowering plants: Evolution above the species level*, Arnold Press, London, pp. 1 – 399.

Chapters from a book

[19] Schafer, H. and Muyzer, G. (2001) Denaturing gradient gel electrophoresis in marine microbial ecology. In *Methods in Microbiology* (Ed. Paul, J. H.), Academic Press, London, Vol. 30, pp. 425 – 468.

Thesis or other diplomas

[21] Nayaka, S. (2004) *The visionary studies on the lichen genus Lecanora sensu lato in India.* Ph. D. Thesis, Dr. R. M. L. Avadh University, Faizabad, India.

Conference proceedings

[4] Mohapatra, G. C. (1981) Environment and culture of early man in the valley of rivers Chenab and Ravi, western sub-Himalayas. In *Proceedings X Congress of IUPPS*, Mexico, pp. 90 – 123.

Online documentation

[9] Koning, R. E. (1994). Home Page for Ross Koning. Retrieved 26-6-2009 from *Plant Physiology Information Website*: http://plantphys.info/index.html.

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