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DEPICTION OF VIBRATIONAL ENERGY LEVELS OF POLYMERIC MATERIALS

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ABSTRACT

Studies of vibrational energy levels of molecules deal with the Infrared spectroscopy. Which is one of the most powerful analytical techniques which offer the possibility of chemical identification? Vibrational spectroscopies, including infrared and Raman techniques, are important tools for the characterization of chemical composition, molecular structures, and this technique when coupled with intensity measurements may be used for quantitative analysis. The technique is based on the simple fact that a chemical substance shows marked selective absorption in the infrared region. After absorption of IR radiations the molecule of a chemical substance vibrates at many rates of vibration, giving rise to close packed absorption bands called an IR absorption spectrum which may extend over wide wavelength range. Various bands will be present in IR spectrum which will correspond to the characteristic functional groups and bonds present in a chemical substance is a fingerprint for its identification one of the most important advantages of infrared spectroscopy over the other usual methods of structural analysis such as X-ray diffraction analysis ,electron spin resonance etc. is that it provides useful information about the structure of compounds and can solve many problems in organic chemistry and coordination chemistry .In present paper ,with the help of Infrared spectroscopy conformation of polymer –metal complex formation has been assured that can help to study of polymer as conducting material to prepare polymer electrodes and polymer electrolytes .This research paper will help to prepare polymer batteries. For this purpose polymer, metal-polymer complex like Polyaniline and Polyaniline-Zinc complex have been tested using KBr as reference material with the help of Infrared spectrophotometer.

Keywords*: vibrational levels, selective absorption, radiations, Polymer electrolytes, polymer electrodes, peak by peak, degenerate, conformation.*

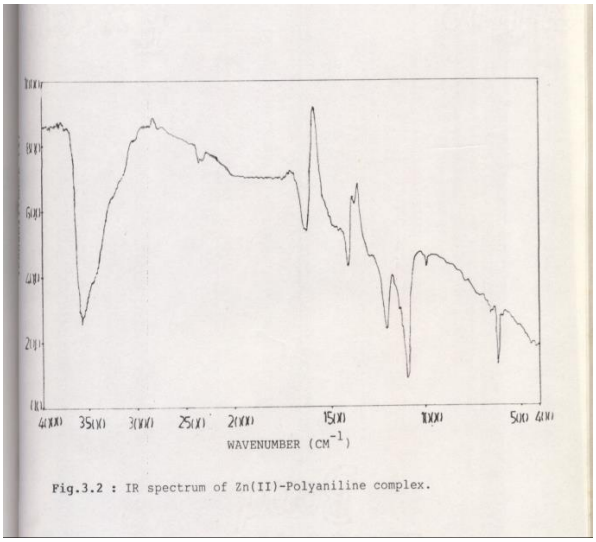
I. INTRODUCTION

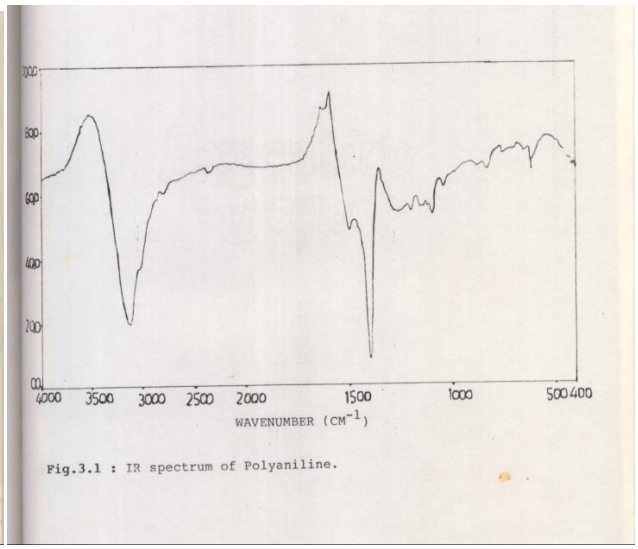
In the past decade intermolecular vibrational energy redistribution (IVR) in isolated molecules has been investigated with good success Vibrational energy flow within and between polyatomic molecules drives chemistry and governs their reactivity. Much less, however, is known about IVR in solution where the intramolecular energy redistribution process is influenced by the surrounding solvent. In a complex polymer molecule the number of infrared transition might be expected to be too great to deal with, but fortunately this does not happen as a great, many of these are degenerate, i.e. of the same energy. The advantage of fingerprint region has been taken in the identification of polymers. The spectrum of the unknown sample is matched against that of an authentic sample, peak by peak, and the identity of the compound established.

Table-Vibrational Frequencies (cm^{-1}) and their assignments for Polymeric Complex s-sharp, m-medium ,w-weak , br-broad

S.No.	Ligand	Assignment	Zn-(II)- PANI Complex
1	3500 ˉI br	-NH stretching	3565
2	3300_I	vibration	-
3	1600w	-C=C	1626
4	1500s	-NH-bending	-
5	Aromatic nature	-	-
6	1380 ˉI br	-C-N vibration	-
7	1360_I	aromatic secondary	1402
8	amine	-	-

9	1100m	CH in plane stretching	-
10	780 -I br	CH bending	-
11	620_I	vibration	619





IR Spectra of Polyaniline –original formate IR spectra of PANI-Zinc complex-original format

II. SURVEY OF LITERATURE

Infrared spectrum of Polymer such as PolyAniline and its 1/1 blend with PAA : at 25° c before heating and at 25°c after heating to 80°c and other various conditions have been reported by Show-An andHsun-Tsinglee,1. They concluded that for the PANI (termed PANI/PAA blend), the confinement of carboxylic acid group.

Ming Xiang of China studied Infrared of PVAL(OH,47mol)/PMMA[2] .He concluded that relatively strong Intermolecular Hydrogen bonding interaction exists between components in the miscible blends. The curve resolving studies of FTIR spectra have suggested that the weakly self associated hydroxyl groups in polyvinyl acetals are liable to form hydrogen bonds with carbonyl groups in PMMA. IR spectra of Copolymer and blend of bismaleimides with phenol alkyl resin (KBr), have been reported by Liu Quingmin Xingxian[3].

III. RESULTS AND DISCUSSION

IR Spectra of Polyaniline and its complex with Zinc (II)metal ion has been depicted in figure . The important Infrared signal and their group assignments have been tabulated in table.

A perusal of the figure and table reveals that the signals due to NH-stretching vibrations at 3500-3300cm^{-1} and –CN aromatic vibration in the ligand spectra undergoes a shift in the spectrum of Zn(II)-PANI complex indicating the involvement of –NH nitrogen complex formation.

IV. CONCLUSION

With the help of Infrared Signals obtained it has been confirmed that complexation of metal like Zn and Aluminum with the polymeric material such as Polyaniline, Polyethene etc. occurs using the general mechanism of complexation which can help to study the polymer as conducting material to prepare polymer electrodes and polymer electrolytes. Hence these results will help to apply these complexes in polymer batteries.

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