Ain Shams University

Faculty of Women for Arts, Science and Education

Physics Department

Preparation and Characterization of Some Polymer Blend

A Thesis

Submitted for the Requirements of

The M.Sc. Degree in Physics

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Ain Shams University,

Submitted By

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Ain Shams University

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Approval Sheet

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The M.Sc. Degree in Physics

This thesis has been approved by supervisor committee

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List of Publications

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Published papers

1 Badry, R., El-Khodary, S., Elhaes, H., Nada, N. and Ibrahim, M., NanoBioLetters, On the molecular modeling analyses of sodium carboxymethyl cellulose treated with acetic acid, 2019, 8(2). pp. 553-557.

2 Badry, R., El-Khodary, S., Elhaes, H., Nada, N. and Ibrahim, M., 2019. The Influence of Moisture on the Electronic Properties of Monomer, Dimer, Trimer and Emeraldine Base Sodium Carboxymethyl Cellulose. *Egyptian Journal of Chemistry*, *62*(The First International Conference on Molecular Modeling and Spectroscopy 19-22 February, 2019), pp.39-56.

In progress

1 Badry, R., Elhaes, H., Nada, N. and Ibrahim, M., Density Functional Theory Study of the Electronic Properties of Solid Polymer Electrolytes based on blends of CMC, PEO and acetic acid

2 Badry, R., Elhaes, H., Nada, N. and Ibrahim, M., Acetic Acid Effect on the Optical, Structural, Electrical and Thermal Properties of Plasticized Sodium Carboxymethyl Cellulose

3 Badry, R., Elhaes, H., Nada, N. and Ibrahim, M., Investigations of the Spectroscopic, Conductivity and Dielectric Properties of Plasticized Solid polymer Electrolytes Based on Blends of Carboxymethyl Cellulose Sodium/ Polyethylene Oxide

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Rania Badry Amin Elsayed

Summary

Summary

Carboxymethyl cellulose sodium (CMC), CMC doped with different concentrations of acetic acid, CMCblended with PEO and CMC blended with PEO/acetic acid samples were successfully prepared via the casting technique.

For solid polymer electrodes (SPEs) based on CMC/acetic acid (first group),acetic acid was added toCMC solutions with percentage between 2.5 wt% and 15.0 wt%. The influence of acetic acid on the band structure of CMC was examined by Ultraviolet-Visible Spectroscopy (UV-Vis.). Fourier Transformer Infrared Spectroscopy (FTIR) is utilized to investigate the molecular structure of CMC. Electrical properties of the prepared samples were studied using Electrical Impedance Spectroscopy (EIS). Also the effect of acetic acid addition on the optical properties of CMC is examined as a function of wavelength in the range from 200 -1000 nm using spectrophotometric measurements of the transmittance, T, and reflectance, R, at nearly normal incidence. The data of transmittance and reflectance were analyzed to determine the optical constants (the refractive index, n, and the absorption coefficient α). The absorption analysis has been performed to determine the type of transitions and the optical energy gaps of CMC and CMC/ acetic acid samples. The type of transition was found to be indirect allowed in pure and doped CMC. The value of the optical band gap energy of CMC was decreased as a result of acid addition.

UV-Vis. results indicated that the optical band gap of CMC is decreased with acetic acid addition. FTIR shows the main vibrational bands of pristineCMC and acetic acid. These bands were shifted to the higher wavenumber region upon the addition of acetic acid. This shiftindicates the formation of hydrogen bond between CMC and acetic acid. A new absorption band was appeared around 1693 cm^{-1} which attributed topresence of the COO^- group of acetic acid.

AC conductivity and dielectric properties of the samples were studied in temperature range (298-388 K) and frequency range (50Hz -1MHz). AC conductivity of CMC increased with increasingtemperature as well as increasing acetic acid concentration up to 5wt.% and started to decrease with increasingacetic acidconcentration. Activation energy was also calculated and decreased with increasing acetic acid concentration. The results of dielectric constant and dielectric loss decreased with increasing frequency.

For SPEs based on CMC/PEO (second group), CMC was blended with PEO at different concentrations. UV-Vis. spectrophotometer was utilized to determine the optical energy gap, type of transition and some optical parameters like the first group of samples. FTIR was used to predict the presence of different functional groups.AC conductivity, dielectric constant and dielectric loss were determined using EIS technique. The optical energy gap of pristine CMC was found to be decreased as a result of blending with PEO. In all blended samples, the electrons follow an indirect allowed transition between the valence and the conduction bands. The optical band gap energy of the virgin polymers(CMC and PEO)was decreased due to blending.

FTIR shows the characteristic bands of both pure CMC and pure PEO. The characteristic bands of pure CMC were shifted to the higher wavenumber.Also, the intensity of CMC characterization bands decreased with increasing PEO content.

The AC conductivity of CMC and PEO was increased to 1.18E-06 S/cm. Also, it was found that the conductivity obeys the Arrhenius theory. The activation energy was decreased to 0.668eV as a consequence of blending.

The lowest activation energy and the highest AC conductivity obtainedfor the sample of 80 wt% CMC / 20wt% PEO.

For SPEs based on CMC/PEO/acetic acid (third group), the physical properties were improved by the addition of different percentages of acetic acid. The prepared samples are examined using UV-Vis. spectrophotometer, FTIR and EIS. The results of UV-Vis. showed that the amorphousness of pure CMC and that of pure PEO was increased due to blending and hence the optical energy gap was decreased. Results of FTIR analysis indicated that a hydrogen bond was formed between the blended polymers and the protons of the carboxylic group of acetic acid.EIS results showed that the sample named 80 wt% CMC / 20wt% PEO/ 2.5 wt% acetic acid has the highest conductivity (5.58E-06 S/cm) and the lowest activation energy (0.225eV).

Finally, molecular modeling was carried out to confirm the analytical results for the three groups of samples. Density functional theory (DFT) at B3LYB (3-21) G* basis set was used to study the electronic properties of CMC due to the addition of acetic acid and due to blending. Total dipole moment (TDM), HOMO/LUMO energy gap and electrostatic potential (ESP) are incorporated to study the changes that occurred in the electronic properties of the studied structures. The results of TDM, HOMO/LUMO energy gap and ESP indicated that the SPEs based on CMC/acetic acid, CMC/PEO and CMC/PEO/acetic acid are suitable for application in energy storage devices as well as electrochemical devices. Where, the TDM increased, HOMO/LUMO energy gap decreased and electro-negativity increased for the structures under study.

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CHAPTER ONE
General Background on Polymeric Materials and Literature Survey