



PHYSICAL CHEMISTRY 2021

15th International Conference
on Fundamental and Applied Aspects of
Physical Chemistry

Proceedings
Volume II

September 20-24, 2021
Belgrade, Serbia



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The Conference is dedicated to the

*30th Anniversary of the founding of the Society of Physical
Chemists of Serbia*

and

100th Anniversary of Bray-Liebhafsky reaction

**September 20-24, 2021
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Title: Physical Chemistry 2021 (Proceedings) **ISBN** 978-86-82475-40-8

Volume II: ISBN 978-86-82475-39-2

Editors: Željko Čupić and Slobodan Anić

Published by: Society of Physical Chemists of Serbia, Studentski Trg 12-16, 11158, Belgrade, Serbia

Publisher: Society of Physical Chemists of Serbia

For Publisher: S. Anić, President of Society of Physical Chemists of Serbia

Printed by: "Jovan", <Printing and Publishing Company, 200 Copies

Number of pages: 6+388, Format A4, printing finished in December 2021

Text and Layout: "Jovan"

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*15th International Conference on
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Organized by

*The Society of Physical Chemists of
Serbia*

in co-operation with

Institute of Catalysis Bulgarian Academy of Sciences

and

*Borekov Institute of Catalysis Siberian Branch of
Russian Academy of Sciences*

and

University of Belgrade, Serbia:

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MICROWAVE ASSISTED SYNTHESIS OF POLYANILINE/PULLULAN (PANI/PULL) COMPOSITE

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ABSTRACT

Microwave assisted synthesis of polyaniline modified by pullulan (PANI/Pull) composite was performed by aniline oxidation with potassium iodate. The PANI/Pull composite was characterized using ATR-FTIR technique. FTIR spectra confirm presence of both components in PANI/Pull composite. Antimicrobial evaluation of PANI/Pull material performed by using a qualitative disk diffusion method on *Candida albicans* (*C. albicans*) culture showed very high sensitivity to PANI/Pull composite. Observed FTIR and antifungal activity represent a promising results especially for potential biomedical applications of PANI/Pull composite.

INTRODUCTION

Growing interest in modification of conducting polymers with biopolymers is due to the fact that a simple procedure can be used to couple the properties of both, conducting polymers and biopolymers, in order to develop materials with improved characteristics [1]. As a conducting polymer, polyaniline (PANI) has achieved great attention due to its high electrical conductivity, unique redox properties, simple preparation and doping procedure, low cost, and therefore it has found a wide range of applications [1,2]. Besides mentioned, it has been shown that PANI represents a novel antimicrobial agent that is active against a broad range of bacteria and thus has a potential applications in food safety and biomedicine as an infection control coatings [3].

The aim of our work was to modify PANI by pullulan to obtain novel and improved composite. Thanks to pullulan's biocompatibility, non-toxicity, biodegradability and wide range of applicability (as low-calorie food additive, packaging material, usage in target drug therapy, tissue engineering, wound healing etc.) [4,5] this polysaccharide biopolymer seemed to be a good candidate as a potential PANI modifier.

In this paper, MW assisted copolymerization of aniline with pullulan using potassium iodate (KIO₃) as an oxidant was conducted.

METHODS

MW Assisted Synthesis. Microwave synthesis of PANI/Pull composite was performed in CEM reactor (CEM Discover 300-W single mode reactor operating at 2.45 GHz). Since the key part of our experiments was to keep a constant temperature as well as an irradiation power during the synthesis, it was carried out in specially designed double jacket reaction vessel which was connected to an external cooling circulating thermostat. For temperature measurements a fiber optic temperature sensor was used. Also, to achieve uniform temperature, the sample was mixed by magnetic stirring

at 400 rpm. Absorbed MW power, P was calculated from: $P = C \cdot m \cdot (\Delta T/\Delta t)_i$, where C represents heat capacity and its value is approximated with the value for pure water of $4.18 \text{ J/g}^\circ\text{C}$, m is mass of the solution and $(\Delta T/\Delta t)_i$ is estimated from the linear temperature increase throughout initial heating period during which dissipation of heat by the external thermostat was small. From mentioned calorimetric method the absorbed power for 80 W emitted power, P and its standard deviation were calculated from six replicates $P = (10.0 \pm 0.5) \text{ W}$. With this experimental design the temperature of the reaction mixture before addition of aniline was maintained at $(26 \pm 2)^\circ\text{C}$. PANI/Pull composite was prepared by aniline oxidation with potassium iodate. In 12 mL of an aqueous solution of 1.25 M hydrochloric acid, 0.432 g KIO_3 and 0.343 g pullulan (or 70 wt% relative to aniline) were added. After initial heating period and when temperature reached constant value aniline (0.480 mL or 0.490 g) was added to HCl, KIO_3 and pullulan mixture. MW synthesis was carried out for 10 min. The PANI/Pull product was obtained by centrifugation. Product was washed thoroughly with 1.25 M HCl aqueous solution, deionized water and acetone to eliminate impurities and low molecular weight oligomers. The product was dried in oven at 40°C overnight.

FTIR characterization. The ATR-FTIR spectra were recorded using Thermo Scientific Nicolet iS20 FT-IR spectrophotometer. A sample was placed in direct contact with an infrared attenuated total reflection (ATR) diamond crystal. All FTIR spectra were collected in the wavenumber range of $1800\text{--}600 \text{ cm}^{-1}$ by co-adding 32 scans with a resolution of 4 cm^{-1} .

Antimicrobial activity. The qualitative antimicrobial evaluation of PANI and PANI/Pull materials was performed using a disk diffusion method [6] with reference culture of fungal strain *C. albicans* (ATCC 24433). Fungal inoculum was adjusted to the concentration of $1\text{--}2 \cdot 10^6 \text{ CFU/mL}$, and 100 μL were seeded in Petri dishes containing Malt agar, followed by placing 1 mg of PANI and PANI/Pull materials on top of it. The Petri plates were incubated at 28°C for 48 h.

RESULTS AND DISCUSSION

Obtained PANI/Pull composite was characterized using ATR-FTIR technique. Besides composite, pure PANI was synthesized as well under the same experimental conditions. The characteristic peaks observed in the FT-IR spectra of PANI/Pull composite give valuable information regarding to the possible interactions between pullulan and PANI. At Figure 1. the ATR-FTIR spectra of PANI (a), PANI/Pull composite (b) and pure pullulan (c) is shown. The spectrum of PANI/Pull composite exhibits bands characteristic of PANI as well as of pullulan which confirms the presence of both components in the composite. For pure PANI (Fig. 1(a)), the characteristic bands [2] attributed to C-C stretching quinoid band, C-C stretching benzenoid band, C-N stretching benzenoid band, band of deprotonated PANI and out-of-plane bending vibration of C-H on para distributed ring appear at 1575 , 1492 , 1296 , 1138 and 826 cm^{-1} respectively. The strongest band at 993 cm^{-1} in the spectrum of pullulan (Fig. 1(c)) corresponds to glycosidic linkages [7]. The most prominent changes of the spectrum of the PANI/Pull composite (Fig. 1(b)), in comparison to the spectrum of the pure PANI, is the red shift of peaks at 1575 and 1492 cm^{-1} (quinonoid (Q) and benzenoid (B) ring-stretching vibrations, respectively) to 1554 and 1458 cm^{-1} and the increase in absorption at about 1000 cm^{-1} , due to the presence of pullulan during the polymerization of aniline. Also, the band at 1296 cm^{-1} , observed in the PANI spectrum attributed to C-N stretching of secondary amine, is significantly weakened and shifted to 1287 cm^{-1} in the spectrum of composite. Qualitative antimicrobial evaluation of PANI and PANI/Pull materials was performed using a disk diffusion method on *C. albicans* culture.

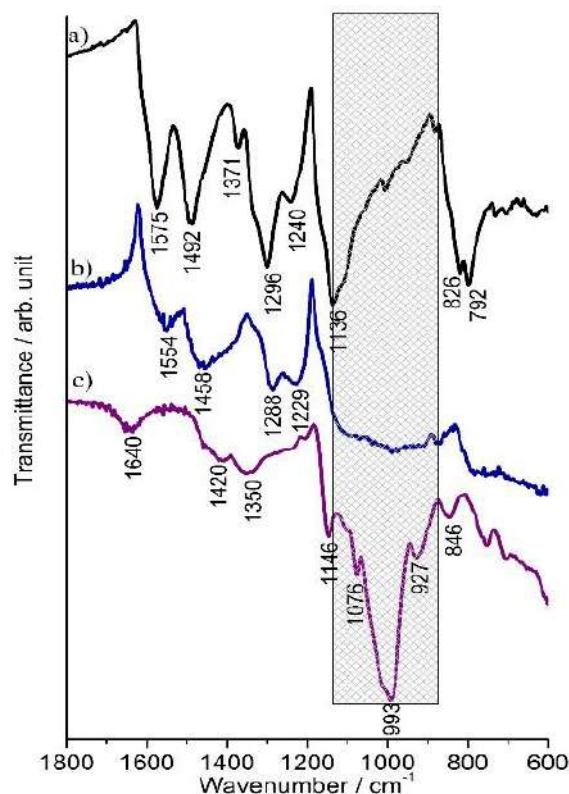


Figure 1. The ATR-FTIR spectra of PANI (a), PANI/Pull composite (b) and pure pullulan (c).

Even though slightly larger inhibition zone was obtained for PANI/Pull composite, obtained results suggest a high sensitivity of *C. albicans* to both PANI and PANI/Pull composite, indicating the antifungal activity of novel material.

CONCLUSION

PANI/Pull composite was synthesized by MW assisted method under constant irradiation power and temperature. FTIR spectra confirmed the presence of both components, pure PANI and pullulan, in the PANI/Pull composite. Qualitative antimicrobial test showed that PANI/Pull has a high antifungal effect against *C. albicans*. Even though obtained results from FTIR and antimicrobial evaluation are promising, especially for potential biomedical application, further investigations are required.

Acknowledgement

This work was partially supported by Ministry of Education, Science and Technological Development of Republic of Serbia (Grant No: 451-03-9/2021-14/200146, 451-03-9/2021-14/200168, 451-03-9/2021-14/200026)

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CIP - Каталогизација у публикацији
Народна библиотека Србије, Београд

544(082)

66.017/.018(082)

502/504(082)

343.98(082)

**INTERNATIONAL Conference on Fundamental and Applied Aspects of Physical Chemistry
(15; 2021; Beograd)**

Physical Chemistry 2021: proceedings: the Conference is dedicated to the 30th Anniversary of the founding of the Society of Physical Chemists of Serbia and 100th Anniversary of Bray-Liebhafsky reaction. Vol. 2 / 15th International Conference on Fundamental and Applied Aspects of Physical Chemistry, September 20-24, 2021, Belgrade, Serbia; [organized by The Society of Physical Chemists of Serbia in cooperation with Institute of Catalysis Bulgarian Academy of Sciences ... [et al.]]; [editors Željko Čupić and Slobodan Anić]. - Belgrade: Society of Physical Chemists of Serbia, 2021 (Belgrade: Jovan). - VI str., str. 347-732: ilustr.; 30 cm

Tiraž 200. - Bibliografija uz svaki rad. - Registar.

ISBN 978-86-82475-39-2

ISBN 978-86-82475-40-8 (niz)

а) Физичка хемија -- Зборници б) Наука о материјалима -- Зборници в) Животна средина -- Зборници
г) Форензика -- Зборници

COBISS.SR-ID 53325065