

## SPECTROSCOPIC ANALYSIS OF THIN FILMS FABRICATED FROM BENZANTHRONE LUMINESCENT DYE

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### ABSTRACT

Thin films samples of organic luminophore - 3-N,N-diacetylaminobenzanthrone deposited on glass substrate were prepared by thermal evaporation obtaining thin films of 2.5 to 3  $\mu\text{m}$  thickness. The structural and spectroscopic properties of obtained films were investigated by confocal microscope with input of femtosecond laser radiation, X-ray diffractometer and scanning electron microscope. It was found that prepared films are highly ordered materials with molecular layers; X-ray diffraction analysis indicate that the distance between these layers is  $\sim 6.5$  Å. In addition, quantum chemical calculations were performed, indicating electron properties of studied dye molecule in ground and excited state.

**Key words:** thin films, luminescent dye, X-ray diffraction analysis, SEM image, quantum chemical calculation

### INTRODUCTION

The design and development of organic molecular materials with high luminance efficiencies in condensed phase is an important contemporary challenge [1]. Organic molecules formed by a donor-acceptor pair connected to a  $\pi$ -delocalized framework present a variety of interesting optical and photoelectric properties [2], therefore these substances are widely used as perspective photoactive materials in optics and optoelectronics [3-6].

Benzo[de]anthracen-7-one dyes are well known as organic luminophores that emit in the spectral region from green to red, depending on the nature of substituents and its conjugation with carbonyl group through a  $\pi$ -system. Because of their bright luminescence, good color characteristics and high thermo and photostability these compounds are used also as disperse dyes, daylight fluorescent pigments and laser dyes [2, 7].

The goal of research presented herein is to investigate the spectral and structural properties of thin films obtained by thermal evaporation of benzo[de]anthracen-7-one derivative - 3-N,N-diacetylaminobenzanthrone, which have potential for use in a number of different fields.

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### METHODS OF SAMPLE MANUFACTURING AND ANALYSIS

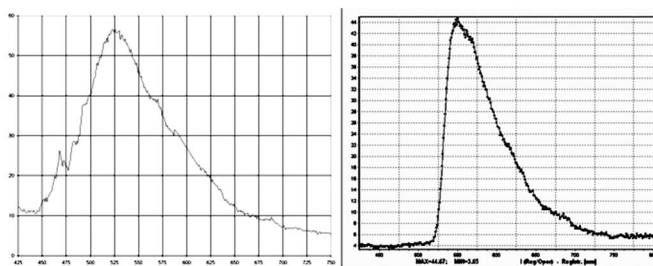
Thin films deposited on glass substrate were prepared by thermal evaporation at vacuum obtaining of the films of 2.5 to 3  $\mu\text{m}$  thickness. Luminescence spectra of films were carried out with confocal microscope Leica LSM TCSP-5 with spectral resolution 2 nm; the samples were irradiated with He/Ar laser ( $\lambda_{\text{ex}}=458 \text{ nm}$ ). The absorption spectra were obtained using a UV-visible spectrophotometer "Specord's UV/VIS" (spectral resolution 0.1 nm). For X-ray analysis was used X-ray diffractometer Rigaku. Scanning electron microscope (SEM) Tescan was used for investigations of prepared film surface.

The fully geometry optimization of the isolated molecule in ground state were optimized using the semiempirical AM1 and PM6 methods. From which some physicochemical and structural parameters of molecules in gaseous phase were estimated. The geometry data were obtained from MOPAC 2009 Version 10.006W. Heats of formation, dipole moments and other parameters were extracted directly from the data files following the geometry optimizations.

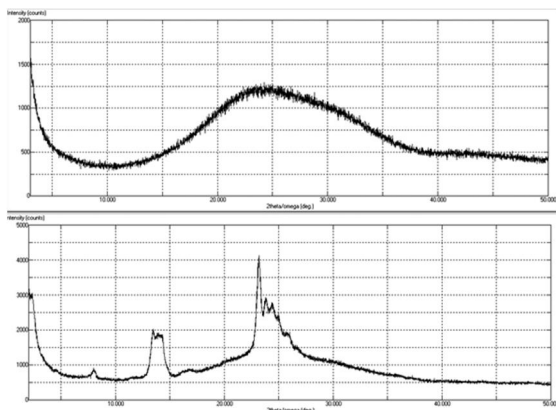
### RESULTS AND DISCUSSION

Spectroscopic and photophysical behavior of the 3-substituted benzantrones is basically related to the polarization of the benzanthrone molecule. The polarization occurring upon irradiation results from the electron donor-acceptor interaction between the electron-donating substituents at the 3-position and the electron-accepting carbonyl group of the chromophorous system [2]. *Figure 1* presents absorption and luminescence spectra of obtained films. The position of absorption maximum is situated at 525 nm, but luminescence maximum – at 550 nm. The Stokes shift is 25 nm, which is smaller than usually for benzanthrone dyes in solvents [8].

This parameter is important characteristic for the luminescent compounds, indicating the differences in the properties and structure of the luminophores molecule between the ground and the first excited state and it is connected with the energy losses during the transition to the excited state.

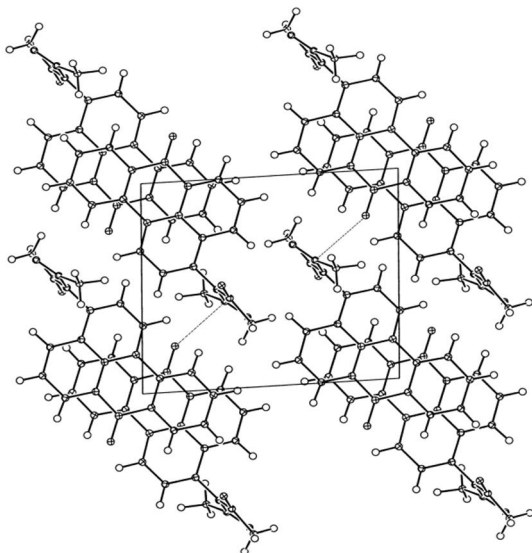


**Fig. 1** – Absorption and luminescence spectra of 3-N,N-diacetylaminobenzanthrone films



**Fig. 2** – X-ray dif-  
fraction analysis of glass  
substrate (up) and 3-N,N-  
diacetylaminobenzanthrone  
films

*Figure 2* presents the results of X-ray diffraction analysis for obtained films. X-ray diffraction analysis indicate that the distance between these layers is  $\sim 6.5$  Å. Similar ordering 3-N,N-diacetylaminobenzanthrone shows in crystal packing (*Fig. 3*).



**Fig. 3** – Crystal structure of 3-N,N-diacetylaminobenzanthrone

The relief images of prepared thin films surfaces were studied by scanning electron microscopy (*Fig. 4*):

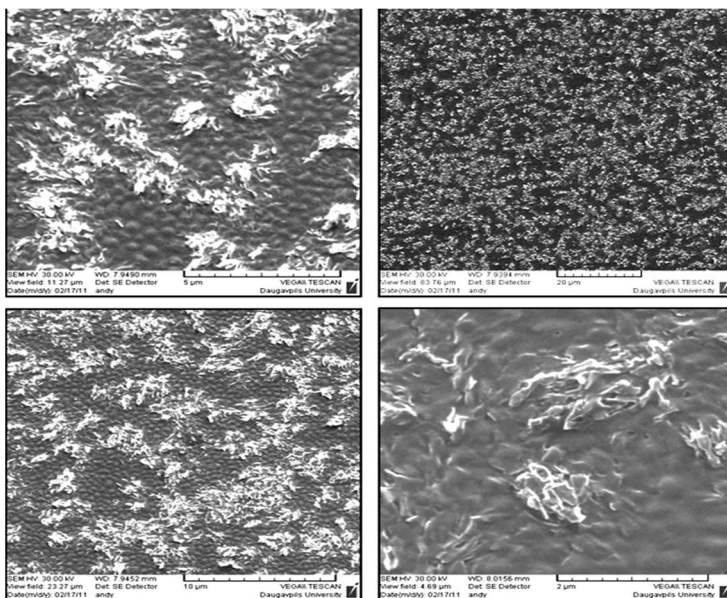


Fig. 4 – SEM images of 3-N, N-diacetylaminobenzanthrone films

The molecular orbital positions are important information for understanding the spectral properties of investigated dye. From quantum chemical calculations can conclude that energy difference in ground and excited state for investigated dye is more than 7 eV.

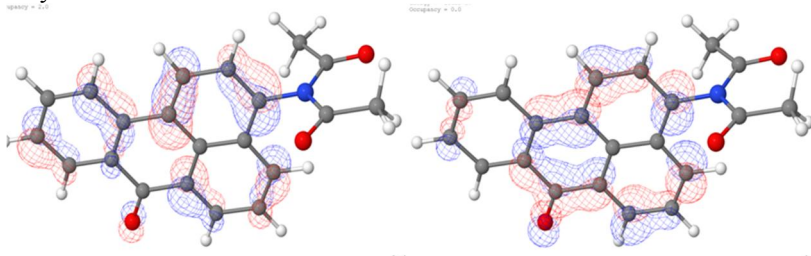


Fig. 5 – Representation of HOMO and LUMO states

### CONCLUSIONS

The prepared thin films of organic luminophore 3-N,N-diacetylaminobenzanthrone show highly ordered structure and demonstrate interesting optical properties.

*Acknowledgements*

This research was supported by the European Structural Funds, Project Nr.2009/0205/1DP/1.1.1.2.0/09/APIA/VIAA/152.

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