

Slovenski kemijski dnevi 2015

Ljubljana, 24. - 25. september 2015



Univerza v Ljubljani
Fakulteta za kemijo in kemijsko tehnologijo



Slovenian Chemical Days 2015

Ljubljana, September 24 - 25, 2015



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FRIT and XRF Study of Wall Paintings Originating From Rila Monastery

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Abstract

This contribution presents a technological study of the wall paintings from Rila Monastery, Bulgaria. The main monastery church - "The Nativity of the Virgin" is painted from the best zographs of The Bulgarian Revival. The works of Dimitar Zograph, Zahari Zograph and Ivan Obrazopisov as iconography and technology were a standard for other painters of the period. Samples were taken from the frescoes in the altar area of the church painted in the period 1841- 1842 year.

Attenuated Total Reflectance Fourier transform infrared spectroscopy (ATR-FTIR) and X-Ray fluorescence analysis (XRF) were applied in order to identify the composition of the painted layers and to determine the employed painting techniques. Combining the XRF and IR data, the following pigments were identified: lime wash, yellow and red ochre, Schweinfurt green, and ultramarine. In all cases, except for the blue paint, egg was used as organic binder. The ATR-FTIR spectra of the blue paint show that it contains a polysaccharide binder instead of egg. The provided useful information on the pigments, organic binders and fillers indicate that the technique of egg tempera painting was employed exclusively, with additional application of the blue colour layer mixed with polysaccharide binder.

Key words: Rila Monastery, pigments, binders, ATR-FTIR, XRF.

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Applicability of ATR-FTIR spectroscopy to distinguish between parchments prepared in different ways

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Abstract

As part of an ongoing study on the parchment making in Byzantium, a large collection of parchment samples was created following the instructions preserved in 5 Armenian manuscripts, dating from the 17th and the 18th centuries, but believed to represent much older tradition widely used in the Byzantine east.

Besides the general steps of parchment making described in other mediaeval literary sources, the Armenian recipes mention some additional operations that include treatments for making the parchment softer and the application of various surface coatings. The materials used for softening are yogurt, bran or pigeons' dung. Rubbing barley flour on the grain side of the wet skins is also mentioned for the same purpose. As final step of the preparation process, almost all recipes recommend the application of different organic coatings and/or lime. The described organic coatings include, flax seed water extract, egg white, combination of both or a mixture of gum, fish glue and alum.

The present contribution reports the ATR-FTIR analysis of selected samples from the collection. The aim of the study was to obtain IR spectral characteristics for each type of parchment and test the applicability of the ATR-FTIR spectroscopy to distinguish between them. For this purpose, parchments treated in four different ways and coated with lime wash, lead white, egg white, flax seed water extract and mixture of gum Arabic, fish glue and alum were tested. Differentiating is challenging due to the complex nature of the spectral information but the use of spectral database with reference materials enables the finding of specific analytical signatures for the different types of treatment that could be used to identify such treatments in real artefacts.

Key words: Byzantium parchments, parchment softening, surface coatings, ATR-FTIR.

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Synthesis and spectral characterization of 3,6-dimethylmorpholine-2,5-dione

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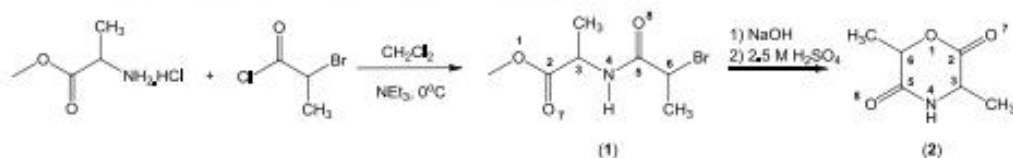
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Abstract

Recently it was demonstrated that cyclodipeptides, comprising in a single α -hydroxycarboxylic acid and an amino acid coupled in a morpholine-2,5-dione ring, show promising pharmacological activities and meet all criteria for good solubility and permeability [1]. In the course of our study, we have focused our attention on the characterization of the most simple among them - 3,6-dimethylmorpholine-2,5-dione, derivative of alanine and lactic acid. Its preparation was achieved by a modification of the method described by in't Veld et al. [2] and allowed isolation of the noncyclic N-(α -bromopropionyl)alanine:



The structures, relative stability of different diastereoisomers and tautomers of both compounds were studied by IR, ¹H and ¹³C NMR spectroscopy and computational DFT methods. The calculated vibrational frequencies and infrared intensities were used to assist the analysis of the experimental IR spectra and describe the changes, accompanying the conversion of the noncyclic N-(α -bromopropionyl)alanine into 3,6-dimethylmorpholine-2,5-dione.

Key words: N-(α -bromopropionyl)alanine, 3,6-dimethylmorpholine-2,5-dione; NMR; vibrational analysis, structure.

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FTIR and DFT Study of the Radical Anion of Dimethyl 3,3'-(5-nitro-2-thioxo-1H-benzo[d]imidazole-1,3(2H)-diyl)dipropionate

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Abstract

Drugs containing a nitroaromatic moiety such as nimesulide, nilutamide, flutamide etc. have been associated with hepatotoxicity due to the formation of hazardous nitroanion radicals, nitroso intermediates and N-hydroxy derivatives [1]. Therefore, in the study of new drug candidates it is important to characterize the potential reductive products of nitroaromatic compounds. The first step in the mechanism of action of nitroheterocyclic drugs as cytotoxic agents for hypoxic cells is the reduction of the nitro group of the drug to the corresponding nitro anion radical [2].

In the course of our study on the hepatotoxicity of substituted 1,3-dimethyl-1H-benzo[d]imidazole-2(3H)-thiones, we generated and characterized the radical anion of dimethyl 3,3'-(5-nitro-2-thioxo-1H-benzo[d]imidazole-1,3(2H)-diyl)dipropionate which shows the highest toxicity within the studied series. The nitro radical anion was electrochemically generated and the spectral and structural changes arising from the conversion were described based on IR spectra and DFT calculations. The structural variations, electron charge distribution over molecular fragments and IR frequency shifting were discussed. The radical anion is characterized by a larger and stronger conjugated system than in neutral form and formation of quinoid-like structure.

Key words: Nitroaromatic drugs, 1,3-dimethyl-1H-benzo[d]imidazole-2(3H)-thiones, radical anion, IR spectra, DFT.

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