It is important to note that in our synthesis no chromatographic purification on the intermediate steps is needed. In addition, a successful use of sunlight as irradiator and air as an oxidant was demonstrated.

1,6-Dihydropyrimidines **3** and pyrimidines **4** were characterized by high resolution ESI⁺-MS, ¹H and ¹³C{¹H} NMR spectroscopy. In addition, the structure of one of dihydropyrimidines was elucidated by a single-crystal X-ray diffraction.

References

- 1. Chen J., Meng H., Zhang F. et al. // Green Chemistry. 2019. Vol. 21. P. 5201–5206.
- Mondal R., Sinha S., Das S. et al. // Advanced Synthesis and Catalysis. 2020. Vol. 362. P. 594–600.

* This work was done under support of the RSF (grant 19-73-10090) using resources of the Magnetic Resonance Research Centre, Chemical Analysis and Materials Research Centre, Centre for X-ray Diffraction Studies of the Research Park of St. Petersburg State University.

УДК 547

V. V. Permikin¹, E. V. Shadrina¹, N. P. Evstigneeva², M. M. Kokhan², T. G. Khonina^{1, 3}

¹Postovsky Institute of Organic Synthesis, Russian Academy of Sciences (Ural Branch), 620990, Russia, Ekaterinburg, S. Kovalevskoy / Akademicheskaya St., 22 / 20, vasiliy_permikin@mail.ru, ²Ural Research Institute for Dermatology, Venereology and Immunopathology, 6200768, Russia, Ekaterinburg, Shcherbakova St., 8, ³Ural State Agrarian University, 620075, Russia, Ekaterinburg, K. Libknekhta St., 42

MECHANISM OF STRUCTURAL NETWORKING IN BIOACTIVE SILICON–ZINC–BORON-GLYCEROL HYDROGEL*

Keywords: sol-gel synthesis, silicon-zinc-boron-glycerol hydrogel, nanoscale structure, mechanism, antimicrobial activity.

Using the sol-gel process, we early synthesized bioactive element-containing hydrogel based on silicon, zinc, and boron glycerolates as biocompatible precursors [1]. It was shown that silicon-zinc-boron-glycerol hydrogel (Si-Zn-B-gel) is

non-toxic, exhibited wound-healing and antimicrobial activity, comparable to commercial drugs (3 % Tetracycline Ointment and 1 % Exoderil Solution). The gel can be used as independent medicines for topical application and as drag delivery system.

The aim of this work was the investigation of the gelation mechanism and structural features of Si-Zn-B–gel that provides the high antimicrobial activity.

Structural features of hydrogel were studied using advanced physicochemical methods. It was shown that the gel 3D-network is formed by the products of hydrolysis and subsequent (co)condensation of silicon and boron glycerolates and includes Si–O–Si and Si–O–B fragments (with residual glyceroxy groups at silicon atoms as result of incomplete hydrolysis of silicon glycerolates in glycerol excess). The main part of zinc monoglycerolate does not undergo the hydrolytic transformations under gelation conditions and exists in the cells of the 3D-polymeric network in the form of amorphous nanoscale particles. Zinc monoglycerolate is not linked to the network by covalent bonds, and it forms a separate phase. TEM micrograph of the sample obtained by drying of a suspension of Si-Zn-B–gel in ethanol on a copper grid does not show crystallinity.

It has been shown by atomic emission spectrometry that a certain amount of zinc (23 wt. % of the initial amount in the gel) is presented in the dispersion medium of Si-Zn-B–gel, which was isolated by exhaustive cold extraction with absolute ethanol. Using electrospray ionization mass spectrometry and ¹¹B NMR, it was found that a dispersion medium of Si-Zn-B–gel contained water-soluble product of combined hydrolytic transformations of zinc and boron glycerolates, namely zinc bis(glycerol)borate Zn[B(C₃H₆O₃)₂]₂.

The formation of $Zn[B(C_3H_6O_3)_2]_2$ can be illustrated by the following general scheme:

$$H_2O$$

ZnC₃H₆O₃ + 2 H[B(C₃H₆O₃)₂] \longrightarrow Zn[B(C₃H₆O₃)₂]₂ + C₃H₈O₃

We have shown that the reaction takes place only in the presence of water and probably proceeds as follows:

$$ZnC_{3}H_{6}O_{3} + 2H_{2}O \xrightarrow{H^{+}} Zn(OH)_{2} + C_{3}H_{8}O_{3}$$
$$Zn(OH)_{2} + 2H[B(C_{3}H_{6}O_{3})_{2}] \xrightarrow{} Zn[B(C_{3}H_{6}O_{3})_{2}]_{2} + 2H_{2}O$$

We believe that the $ZnC_3H_6O_3$ partial hydrolysis catalyzed by $H[B(C_3H_6O_3)_2]$ acid with the formation of $Zn(OH)_2$ takes place during the formation of Si-Zn-B–gel. Then $Zn(OH)_2$ interacts with $H[B(C_3H_6O_3)_2]$ to form $Zn[B(C_3H_6O_3)_2]_2$ complex salt that is an aqueous solution as the Zn^{2+} cations and bis(glycerol)borate anions $[B(C_3H_6O_3)_2]^-$.

The simultaneous presence of these ions, in our opinion, provides the increased antimicrobial activity of Si-Zn-B–gel in comparison with silicon–boron- [1, 2] and silicon–zinc-glycerol [1,3] hydrogels. Thus, Si-Zn-B–gel can be an efficient and safer alternative to conventional topical antimicrobial agents for treatment of diseases of skin and mucous membrane.

References

- 1. *Khonina T. G., Chupakhin O. N., Kungurov N. V. et al.* // Russian Chemical Bulletin. 2019. Vol. 68. P. 1621–1628.
- Chupakhin O. N., Khonina T. G., Kungurov N. V. et al. // Russian Chemical Bulletin (Int Ed). 2017. Vol. 66, № 3. P. 558–563.
- 3. *Khonina T. G., Ivanenko M. V., Chupakhin O. N. et al.* // European J. of Pharmaceutical Sciences. 2017. Vol. 107. P. 197–202.

* This work was carried out in the framework of the Russian State Assignment (theme № AAAA-A19-119011790134-1).

УДК 615.012.1

K. V. Savateev¹, E. N. Ulomsky¹, V. L. Rusinov¹, O. N. Chupakhin², V. N. Charushin², I. M. Sapozhnikova¹, S. K. Kotovskaya¹, R. A. Litvinov³, D. A. Babkov³, A. A. Spasov³

¹Ural Federal University, 620002, Russia, Ekaterinburg, Mira St., 19, ²Institute of organic synthesis named after I. Ya. Postovskiy, 620137, Russia, Ekaterinburg, S. Kovalevskoy St., 20, ³Volgograd state medical university, 400131, Russia, Volgograd, Pavshikh Bortsov St., 1, i-krafttt@yandex.ru

NEW ANTIGLYCATING AGENTS FOR DIABETES THERAPY*

Keywords: azolopyrimidines, azolotriazines, antiglycation, antidiabetic, dipeptidyl peptidase-4.

In 2015, there were an estimated 415 million people diagnosed with DM in the world. DM disability and mortality are directly associated with late vascular