

## HEXAFLUOROSILICATES WITH ANTIBACTERIAL CATIONS

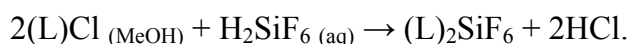
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The "onium" hexafluorosilicates, in particular, ammonium hexafluorosilicate  $(\text{NH}_4)_2\text{SiF}_6$  and hexafluorosilicates of amino acids represent in the recent years the objects of intensive research as compounds possessing by the caries-protected and hyposensitive properties [1-3]. In present communication we describe some results of synthesis and physico-chemical investigations of three new salts with antibacterial cations –  $(\text{CH})\text{SiF}_6$ ,  $(\text{PHMG})(\text{SiF}_6)_{1.5}$  and  $(\text{CP})_2\text{SiF}_6$  (CH – chlorhexidine, PHMG – polyhexamethylene guanidinium, CP – cetylpyridinium).

The compounds with the composition  $(\text{CH})\text{SiF}_6$  (**I**),  $(\text{PHMG})(\text{SiF}_6)_{1.5}$  (**II**) and  $(\text{CP})_2\text{SiF}_6$  (**III**) were obtained by the interaction of corresponding "onium" chlorides in methanol solution with fluorocomplex acid  $\text{H}_2\text{SiF}_6$  (45 %) in mole ratios 1 : 3 [4]:



Reaction products **I** – **III** were isolated in an approximately qualitative yield. All compounds were characterized by elemental analysis, IR, NMR  $^{19}\text{F}$  and mass-spectrometry. Mass spectra (EI) of **I** – **III** are contained the peak of ion  $[\text{SiF}_3]^+$  ( $m/z = 85$ ) – characteristic product of fragmentation of  $\text{SiF}_4$ . According to IR spectroscopy data, "onium" hexafluorosilicates **I** – **III** have ionic structures. The vibrations of the groups  $\nu(\text{NH})$ ,  $\nu(\text{N}^+\text{H}_2)$  in the salts **I** and **II** appear as a strong absorption bands at  $3360 - 3180 \text{ cm}^{-1}$ ;  $\delta(\text{N}^+\text{H}_2)$  vibrations appear at  $1634$  and  $1637 \text{ cm}^{-1}$ . In compound **III**, three  $\nu_{\text{ring}}$  vibrations at  $1638$ ,  $1577$  and  $1488 \text{ cm}^{-1}$  are observed. The strong  $\nu(\text{SiF})$  and  $\delta(\text{SiF}_2)$  stretches of  $\text{SiF}_6^{2-}$  anions are observed in their characteristic regions (at  $744 - 734$  and  $482 \text{ cm}^{-1}$  respectively). The NMR  $^{19}\text{F}$  spectra of compounds **I**, **II** (d-DMSO) and **III** ( $\text{CDCl}_3$ ) have one resonance at  $-136.70$ ,  $-135.09$ ,  $-133.8$  ppm. The range of chemical shifts observed could be due to changes in sample concentration, different solvents, the presents or absents of water, and the differing cationic species.

The results of thermogravimetric analysis are consistent with a multi-stage thermolysis scenario for hexafluorosilicates **I** and **II**. The temperatures of thermolysis beginning of the complexes **I** and **II** are  $270$  and  $100 \text{ }^\circ\text{C}$ , respectively. The studied compounds **I** – **III** are characterized by the predicted high tendency to hydrolysis in dilute aqueous solutions with the formation of silica and fluoride anion that allows considering these salts as potential caries-protected agents. The study of biological activity of these compounds is the subject of further investigations.

### References

1. T. Suge, A. Kawasaki, K. Ishikawa et al., Dent. Mater. 24 (2008) 192-198.
2. T. Suge, A. Kawasaki, K. Ishikawa et al., Dent. Mater. 26 (2010) 29-34.
3. N.A. Brsikyan, L.H. Andriasyan, G.R. Badalyan et al., The New Armenian Med. J. 6 (2012) 52-55.
4. V.O. Gelmboldt, V.Yu. Anisimov, O.V. Prodan, Ukrainian patent № 84762 (2013).