Interaction of silver clusters with dioxidine molecules within hybrid nanocomposites obtained by cryocondensation from the gas phase

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The creation of hybrid systems based on antibacterial drugs with metal nanoparticles is a promising direction in the field of rational drug design. The addition of silver nanoparticles to antibacterial drugs has been shown to increase the antibacterial activity of the entire system due to the synergistic action of its components [1]. A further development of this approach is the formation of more complex structures, including silver nanoparticles in the matrix of drug, which may contribute to additional localization of the joint action of components. In such structures, the role of drug molecule contacts with clusters and metal nanoparticles increases significantly, which affect the spectral and physical properties of the entire sample [2].

In this study, nonempirical calculations of complexes of the antibacterial drug dioxidine with silver clusters of different sizes (Ag_n, n = 1–3, 13) are carried out using DFT/B3LYP5 theory and GAMESS (US) quantum chemistry package. Dioxidine has been shown to have two main coordination centers in complexes with silver: oxygen hydroxyl and nitroxyl groups. The obtained theoretical data on the geometry and energy of the dioxidine-silver complexes were compared with experimental data, including the IR spectra of the samples of hybrid dioxidine-silver nanocomposites obtained by the method of cryocondensation from the gas phase [3]. It was shown that the shift and broadening of bands in the IR spectrum can be caused both by the influence of a polymorphic triclinic structure and by the interaction of a molecule with silver clusters, and in the latter case, the observed shifts of bands corresponding to oscillations in N-O and C-OH bonds confirm the conclusions of theoretical calculations on the two coordination centers of dioxidine and reflect the dissociation energy ratios of the corresponding complexes.

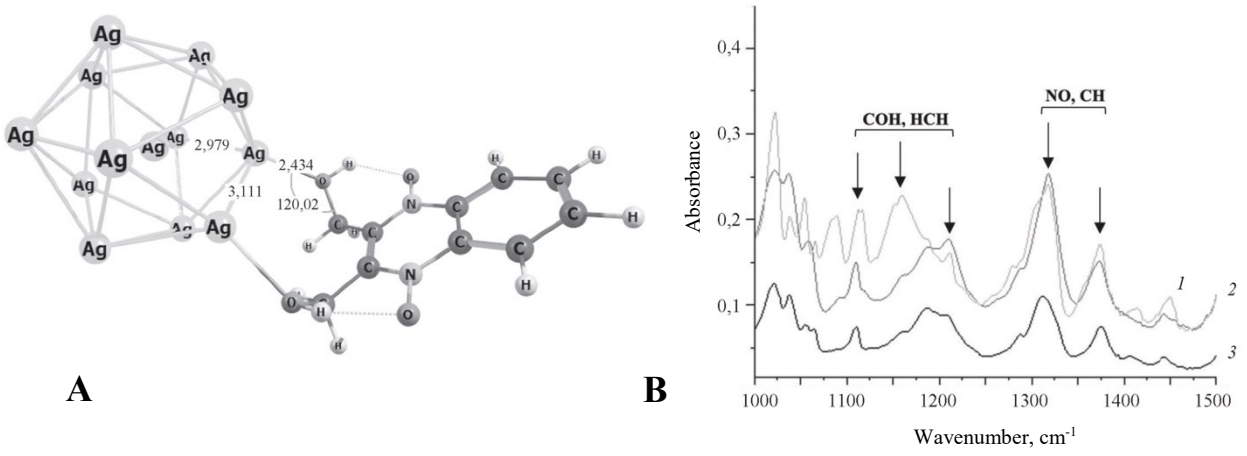

Fig. 1. A – the structure of dioxidine-Ag_{13} complex; B - a fragment of the IR spectrum of dioxidine samples (1 – pharmacopeia dioxidine, 2 – dioxidine nanoforms (T form), 3 – hybrid nanocomposites of dioxidine with silver)

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