

Complex Formation of 1,5-Bis(amidomethylsulfonyl)pentane with Copper(II) and Iron(III)

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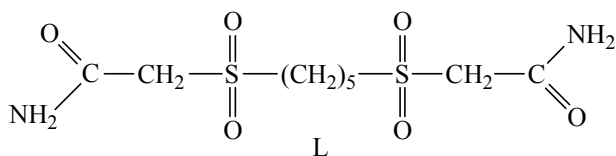
Abstract—The state of the new antitubercular agent 1,5-bis(amidomethylsulfonyl)pentane in aqueous micellar solution of the nonionic surfactant Bridge 35 and its complexing properties toward copper(II) and iron(III) ions have been studied by spectrophotometry, pH potentiometry (25°C, variable ionic strength), and mathematical modeling. In the concentration range from 5.00×10^{-5} to 1.00×10^{-3} M in the presence of Bridge 35, the title compound exists in a neutral monomeric form. It forms 1:2 mononuclear and 2:2 binuclear complexes with copper(II) and 1:1 and 1:2 mononuclear and 2:1 binuclear complexes with iron(III). The most favorable structures of 1,5-bis(amidomethylsulfonyl)pentane and its complexes have been simulated in terms of the density functional theory.

Keywords: 1,5-bis(amidomethylsulfonyl)pentane, copper(II), iron(III), complex formation, ligand denticity

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Directed synthesis of compounds exhibiting anti-tubercular activity and study of their physicochemical properties are quite important problems. The data on the behavior of compounds in solution can be used to predict biological consequences of metabolism of a particular compound in living organisms. We previously determined quantitative parameters of protolytic equilibria and complex formation reactions in solution for triazine-2,4-diamine derivatives and isocyanurates which possess high antimycobacterial activity and species specificity for mycobacteria [1–4].

1,5-Bis(amidomethylsulfonyl)pentane (L) is a new antitubercular agent synthesized in the Arbuzov Institute of Organic and Physical Chemistry (Kazan Scientific Center, Russian Academy of Sciences [5].



There are no data on the structure, state in solution, and complexing properties of 1,5-bis(amidomethyl-

sulfonyl)pentane and analogous α,ω -bisamides. 1,5-Bis(amidomethylsulfonyl)pentane is poorly soluble in water (2.0×10^{-4} M), but its solubility increases by a factor of 5 (to 1.00×10^{-3} M) in the presence of the nonionic surfactant Bridge 35 at a micellar concentration (1.0×10^{-3} to 1.0×10^{-2} M); the critical micelle concentration (CMC) of Bridge 35 is 6×10^{-5} to 9.1×10^{-5} M [6]. The solubility of 1,5-bis(amidomethylsulfonyl)pentane in 40% aqueous DMSO ($c_{\text{DMSO}} = 5.62$ M) is approximately 60 times higher than its solubility in water and is 1.25×10^{-2} M.

We have studied the behavior of 1,5-bis(amidomethylsulfonyl)pentane in solutions containing Bridge 35 as models of the microheterogeneous medium of an organism (cell membranes, blood, etc.) with the goal of finding out the possibility of complexation of this potential multidentate ligand with copper(II) and iron(III).

Solutions of L containing Bridge 35 ($c_{\text{Br}} = 10^{-3}$ M) are almost neutral (pH 6.50). A solution of 1,5-bis(amidomethylsulfonyl)pentane was titrated with aqueous HCl in the presence of Bridge 35. The