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Modeling of equilibria of formation of mono- and polynuclear heteroligand complexes of nickel(II) with ethylenediaminetetraacetic and 2-amino-3-methylbutanoic acids in aqueous solution

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Abstract

Coordination and protolytic equilibria in binary ternary systems containing nickel(II) salt, ethylenediaminetetraacetic (EDTA) and 2-amino-3-methylbutanoic (valine, HVal) acids were investigated by absorption spectrophotometry at NaClO₄ (I = 0.2, T = 20 °C). The results of mathematical modeling showed that most likely mathematical models for the description of experimental dependencies of absorption on the pH and concentration of components of a solution include dissociation constants for ligands, stability constants for homoligand, heteroligand and polynuclear complexes $[Ni_mVal_nEdta_r]^{2m-n-4r}$ (m = 1-4, n = 0-6, r = 0-1). The equilibrium constants of reactions and the stability constants of resultant complexes have been calculated. The structure of the complex found has been proposed.