COMPLEXATION PROPERTIES OF H-GHKHG-H WITH COPPER(II) STUDIED BY THE DECOMPOSITION OF ANIZOTROPIC EPR SPECTRA

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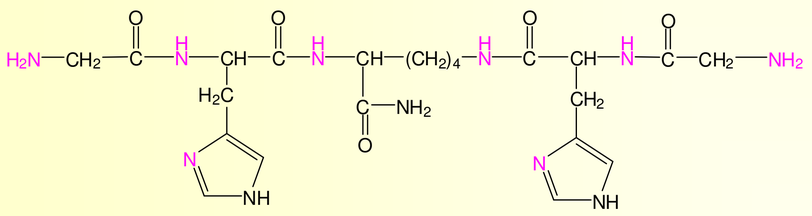
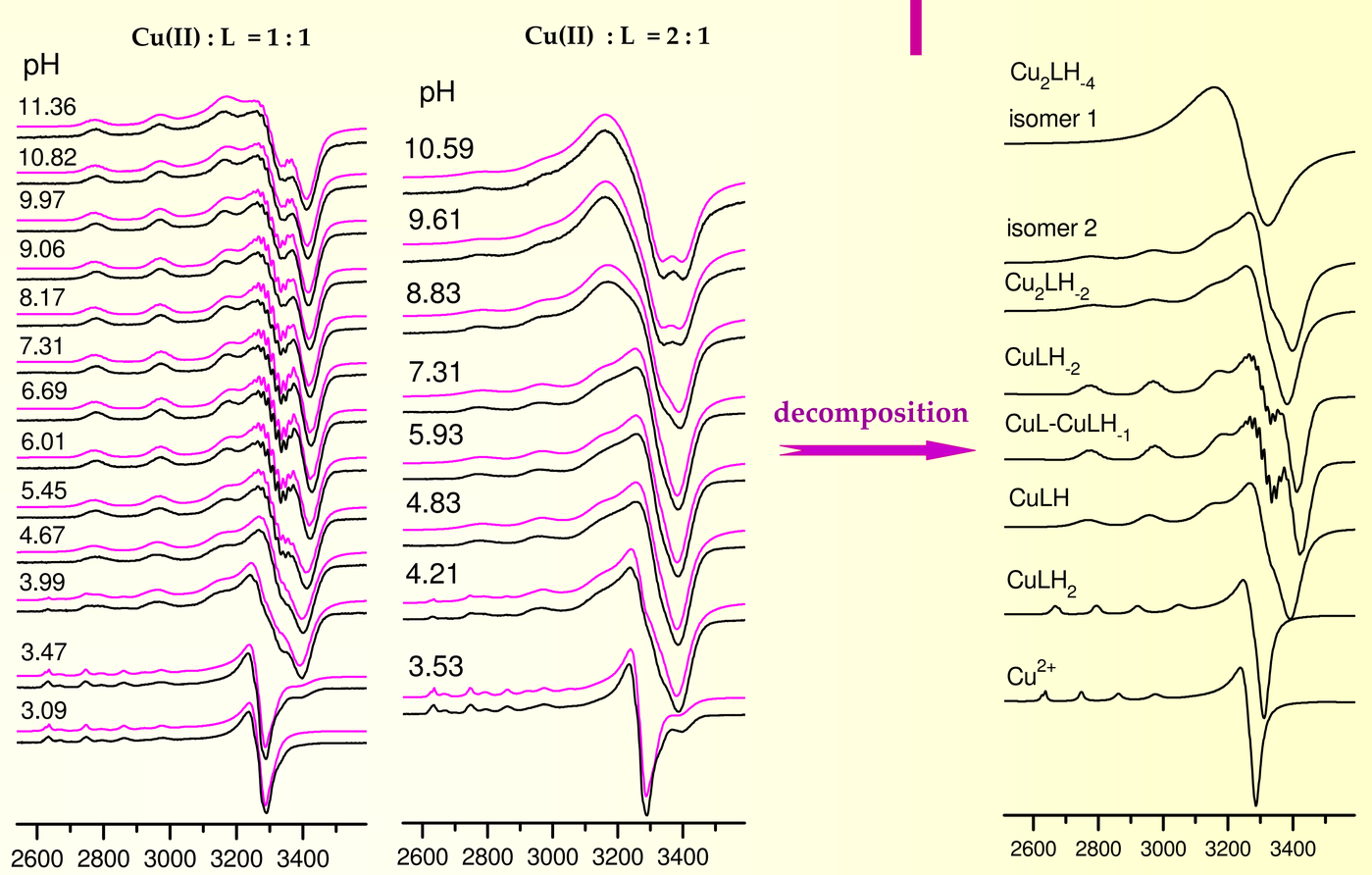
1. Introduction

In several diseases the accumulation of heavy metal ions were established (eg. Al^{3+} accumulation in Alzheimer disease). In these cases the elimination of the metal ions could be a prospective therapy. As a possible therapeutical agent the small oligopeptide H-GHKHG-H was synthesised to produce a ligand with very high complexation feature. Our goal was to investigate the complexation properties of this ligand with copper(II) in aqueous solution at different pH's.



2. Experimental

21 anisotropic EPR spectra were recorded at 77 K at pH range 3-11 in the solutions of T_L = 1mM, $T_{Cu(II)}$ =1mM or 2mM concentrations. EPR spectra were recorded in a dewar containing liquid nitrogen with a BRUKER EleXsys E500 spectrometer (microwave frequency 9.51 GHz, microwave power 12 mW, modulation amplitude 5 G, modulation frequency 100 kHz).



Recorded spectra (black) together with simulations (magenta)

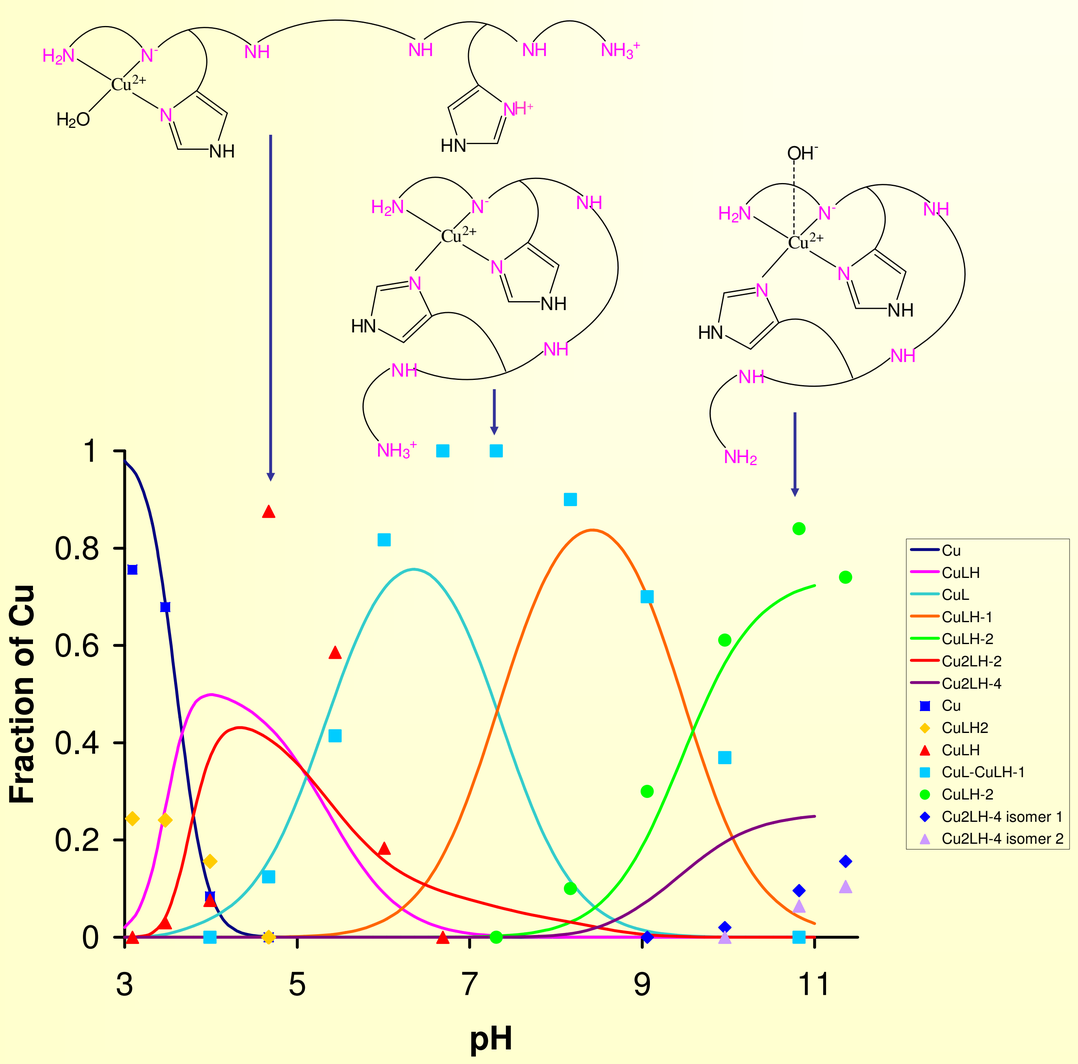
Component spectra obtained by simulation

3. Simulation of EPR spectra

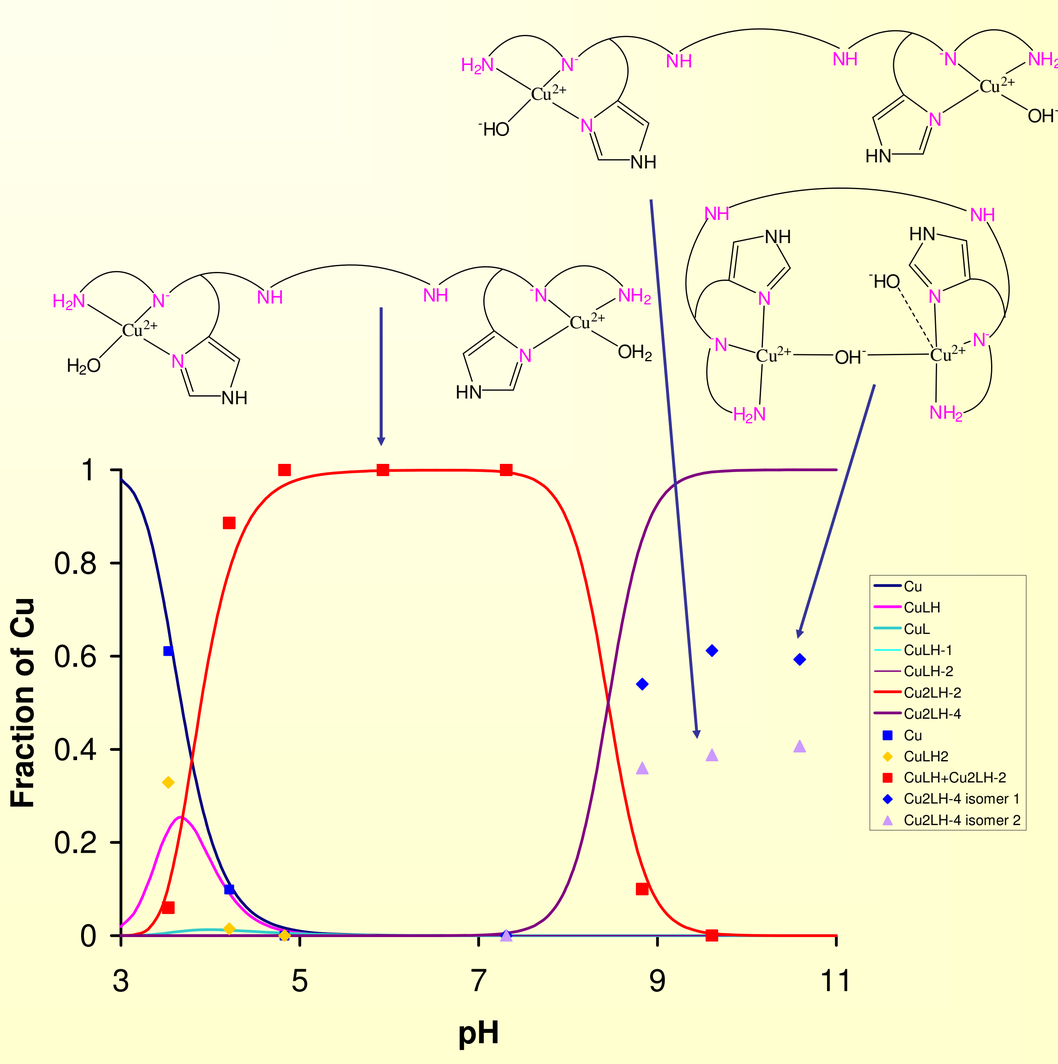
In this overlapping equilibrium system a number of complexes with different compositions and structures are formed by stepwise deprotonation of the donor groups, which necessitates the decomposition of the spectra.

Anisotropic ($g_{||}$, $g_{\perp}$, $A_{||}$, $A_{\perp}$ copper couplings, a_N isotropic nitrogen couplings and orientation dependent linewidth , $W_{MI} = \alpha + \beta M_I + \gamma M_I^2$.) parameters of the components were fitted by the EPR [1] computer program in order to reduce the average square deviation between the experimental and the calculated spectrum. The program is able to take into account maximum three component spectra.

4. Equilibrium model and coordination modes



Cu(II) : L = 1 : 1



Cu(II) : L = 2 : 1

Distrubution curves for obtained from pH-potentiometry (lines) and from the simulation of anisotropic EPR spectra (symbols) together with suggested structures of the complexes.

[1] T. Szabó-Plánka, A. Rockenbauer, L. Korecz, Magn. Reson. Chem. 37, 484-492 (1999)