

## Structure and Dynamics of Solvation Shells of Copper(II) Complexes with N,O-Containing Ligands

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### Abstract

© 2015 American Chemical Society. EPR, NMR relaxation methods, and DFT calculations were jointly used to investigate the structural and dynamical characteristics of solvation shells of copper(II) complexes with iminodiacetic acid, glycylglycine, and glycyglycylglycine in comparison with the copper(II) bis-glycinate studied previously. A strong trans influence of deprotonated peptide nitrogen was revealed in EPR spectra parameters of copper(II) complexes with oligopeptides. With models of the experimental NMRD data and literature X-ray structural information, it was suggested that only one water molecule coordinates in axial position of copper(II) complexes with glycine and di- and triglycine (Cu(Gly)<sub>2</sub>, Cu(GGH-1), and Cu(GGGH-2-)), and the copper ion in these complexes is pentacoordinated, while in the iminodiacetate complex, Cu(IDA), both apical positions can be occupied by solute molecules. The obtained structural results were confirmed by DFT calculations of structures of studied compounds using different functionals and basis sets. It was shown that the donor ability of equatorial ligands and trans influence have an effect on the characteristics of the axial water bond. With increasing donor strength of equatorial ligands, pentacoordination of copper(II) complexes in water solutions becomes more preferable.

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