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Hydration of copper(II) amino acids complexes

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Abstract

© 2017 Wiley Periodicals, Inc. Hydration of the copper(II) bis-complexes with glycine, serine, lysine, and aspartic acid was studied by DFT and MD simulation methods. The distances between copper(II) and water molecules in the 1st and 2nd coordination shells, the average number of water molecules and their mean residence times in the hydration shells were calculated. Good agreement was observed between the values obtained and those found by DFT and NMR relaxation methods. Influence of the functional groups of the ligands and the cis-trans isomerism of the complexes on the structural and dynamical parameters of the hydration shells was displayed and explained. Analysis of the MD trajectories reveals the competition for a copper(II) axial position between water molecules or water molecules and the functional chain groups of the ligands and confirms the suggestion on the pentacoordination of copper(II) in such complexes. MD simulations show that only one axial position of Cu(II) is basically occupied at each time step while in average the coordination number more than 5 is observed.

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Keywords

Amino acids, Copper(II), DFT, Hydration, MD simulation, Pentacoordination