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SERS investigation of neocuproine adsorption on silver: Influence of electrode potential on methyl groups

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Abstract

© 2017 John Wiley & Sons, Ltd. Study of molecules adsorption on charged surfaces is important for biologically relevant substances where the potential at the interface such as living cell membrane is a significant parameter in the processes of their transportation or transmembrane penetration. In this work, a hybrid optical/electrochemical surface-enhanced Raman scattering (SERS) technique was applied to get new insight into the adsorption state and conformational equilibrium of neocuproine, which serves as a nucleic acid biosensor in clinical diagnostics and has biological activity towards several types of carcinoma. The density functional theory calculations performed for several rotational conformations and their anion radicals were used to determine the geometrical and energetic characteristics, to evaluate the rotational barrier, to obtain the vibrational assignment, and to consider the metal-adsorbate charge transfer. The dependence of SERS spectra on surface potential is ascribed to a change of the rotational dynamics of methyl groups from hindered to almost free at potentials ≤-200 mV. It is demonstrated for the first time that SERS spectroscopy is capable to recognize the surface species, which differ in the methyl group internal rotation.

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Keywords

Adsorption, Methyl group, Neocuproine, SERS, Silver electrode