

# Vibrational and theoretical study of azabipiridyl macrocycle and its Ni(II), Cu(II) and Zn(II) complexes deposited onto a smooth copper surface

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The infrared spectra of the azabipiridyl macrocycle complexes of Ni(II), Cu(II) and Zn(II) were registered between 4000 and 200  $\text{cm}^{-1}$ . The spectral assignment allowed to identify the complex formation and structural differences in the coordination site of the complexes. The Ni complex is coplanar to the coordinating N atoms; the copper ion is slightly out of the coordination site plane and the Zn cation is decidedly out of that plane. The stability order of the complex formation  $\text{Ni} > \text{Cu} > \text{Zn}$ , is proposed. Specular reflectance IR spectra indicated that the ligand displays an aleatory orientation onto the smooth copper surface and the Ni and Cu complexes are oriented plane parallel to the surface. The Zn complex-surface interaction is the less energetic in the series. A theoretical study using the INDO/1 semiempirical method and a molecular model for the interacting adsorbate-substrate system support quite well the experimental results and allow an interpretation of the energetic process