Infrared and theoretical interpretation of the structure of naphthalocyanine and its copper(II) complex deposited onto a smooth copper surface

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The infrared spectra of naphthalocyanine (H2Nc) and its copper(II) complex (CuNc) were registered in the region 4000-450 cm-1. These compounds were deposited onto a smooth copper surface and their specular infrared spectra were compared with those of the compounds dispersed in KBr and deposited onto a KBr monocrystal. The differences observed in the spectra of the macrocycle complex were interpreted in terms of slights structural modifications of the macrocycle complex caused by the interaction with the copper surface. The most probable orientation and the energy of the interaction were evaluated through out a simplified molecular model and using INDO/1 and Extended Hückel semiempirical methods.