

Surface Enhanced Raman Spectroscopy (SERS) Study of Diluted Solutions of Cimetidine and Some of its Metallocomplexes

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Cimetidine (**cim**) is a drug used in the treatment of peptic ulcer, and acts as a powerful histamine H₂-receptor antagonist. **Cim** is able to coordinate transition metal ions, and some clinical studies supported the hypothesis that the interaction with metals may play an important role *in vivo* [1]. SERS technique offers the suitable sensitivity to study these interactions at physiological concentrations.

Figure 1 shows the 300–1800 cm⁻¹ spectral region of SERS spectra of **cim** and of **cim**:Me 1:1 complexes. Noticeable differences are observed in the presence of divalent cations, mainly in the 600–1100 cm⁻¹ spectral region, particularly in the case of Cu⁺⁺ ions (d). Also the relative intensity of the bands near 1300 cm⁻¹ changes, with the appearance, in the **cim**:Cu⁺⁺ system, of a new component at 1320 cm⁻¹. Moreover, the ν_{CN} stretching band at about 2200 cm⁻¹ shifts to higher frequency in the presence of copper ions. An ab initio calculation with the HF/6-31G** basis set was performed to estimate the energetic stability consequent to the binding of the different groups of **cim** with Ag surface and used to determine the optimized geometry of **cim** and of **cim**:Me 1:1 complexes adsorbed on the colloid. The SERS and DFT results suggest that the site of adsorption changes. Moreover, they differs noticeably from the Raman spectra of the pure solid crystalline **cim** and of some solid **cim**-Me complexes [2], confirming the great ability of SERS technique to deal with problems related to the biomedical field. Moreover, they support the hypothesis that the copper ion plays an important role in increasing the pharmacological efficacy of **cim**.

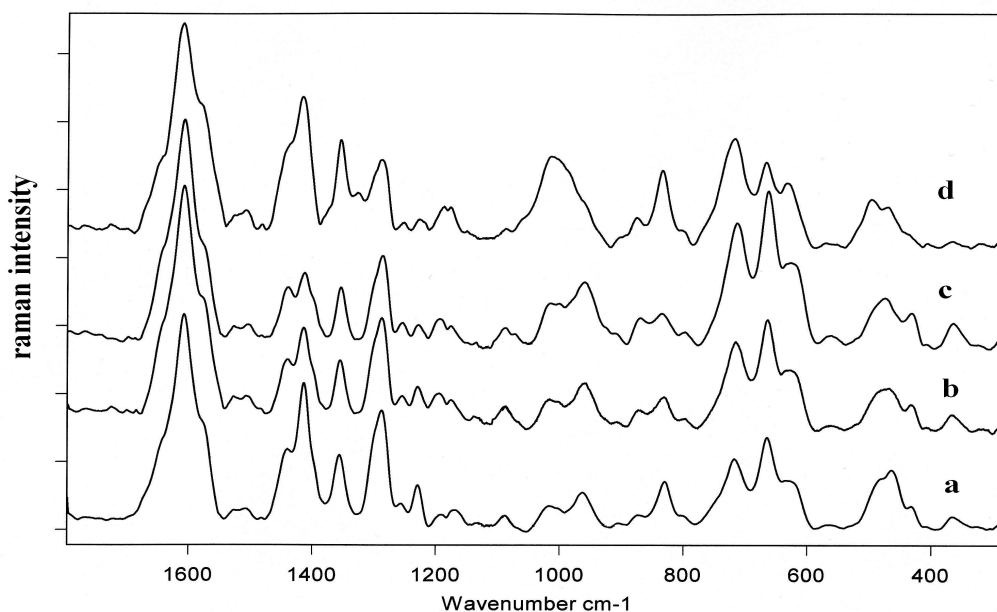


Fig. 1: 300–1800 cm⁻¹ spectral region of SERS spectra of **cim** 0.05 % (a) and of its metallocomplexes (**cim**:Me 1:1) with Ca (b); Cd (c) and Cu (d).

[1] M. Kirkova, M. Atanassova, E. Russanov, Gen. Pharmacol. 33 (1999) 271.

[2] M. Barańska, L.M. Proniewicz, J. Mol. Struct. 511-512 (1999) 153.