

Spectroscopic Investigation of Some Cu(II) Cardiovascular Complexes

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The atenolol (ATE), metoprolol (MET), pindolol (PIN) and verapamil (VER) molecules are most frequently used drugs in the treatment of cardiovascular diseases. They are beta-blocker drugs and reduce the symptoms of angina pectoris (chest pain), decrease the blood pressure of the population with hypertension and are used also in the people treatment after heart attacks. In the last few years, some molecular copper complexes of different drugs (cardiovasculars, antiinflammatories) are used because their activity is enhanced [1-3]. For a better understanding of their activity, structural investigation by different spectroscopic methods (FT-IR, Raman and EPR) and DFT calculations was done.

Molecular complexes with Cu(II) were prepared on going from the starting salts (sodium benzoate and copper sulphate) by co-precipitation procedure. After drying, the powder complexes were analysed by classical KBr pellet technique with an EQUINOX 55 Bruker FT-IR spectrometer in the 400-4000cm⁻¹ spectral domain. FT-Raman spectra were recorded in a backscattering geometry with a Bruker FRA 106/S Raman accessory attached to the FT-IR spectrometer. The EPR spectra of the samples in the powder form were registered in the X band using an ADANI-USA spectrometer.

A comparative study of the FT-IR and Raman spectra of ligands (ATE, MET, PIN and VER) and the corresponding metal complex, allowed us to establish the molecular groups involved in the complexation. In the case of ATE and MET copper compounds, the NH₂ and carboxyl groups are involved in the coordination of the metal ions. Also for PIN and VER compounds the coordination is realized by nitrogen and oxygen atoms from their corresponding molecular groups.

For the assignment of the vibrational bands, density functional theory (DFT) calculations were performed on these molecules. The use of new and rapid instrumentation in IR and Raman spectroscopy has made these techniques suitable for drug process monitoring.

Powder EPR spectra of Cu(II) complexes obtained at room temperature exhibit the absorption signals typical of randomly oriented single state (S=1/2) species having axial symmetry. The ground state for paramagnetic electron is d_{x²-y²} orbital, for ATE, MET and VER compounds. For PIN compound the ground state is d_{z²} orbital. By comparing the shape of these EPR spectra with those obtained for other copper complexes with nitrogen and oxygen ligands we have concluded that the local symmetry around metal ions is of square-planar type with a CuN₂O₂ chromophore in the xOy plane [4].

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