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Physicochemical Investigation of Caffeic Acid and Caffeinates with Chosen Metals (Na, Mg, Al, Fe, Ru, Os)

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Abstract : Caffeic acid (3,4-dihydroxycinnamic) is distributed in a free form or as ester conjugates in many fruits, vegetables and seasonings including plants used for medical purpose. Caffeic acid is present in propolis – a substance with exceptional healing properties used in natural medicine since ancient times. The antioxidant, antibacterial, antiinflammatory and anticarcinogenic properties of caffeic acid are widely described in the literature. The biological activity of chemical compounds can be modified by the synthesis of their derivatives or metal complexes. The structure of the compounds determines their biological properties. This work is a continuation of the broader topic concerning the investigation of the correlation between the electronic charge distribution and biological (anticancer and antioxidant) activity of the chosen phenolic acids and their metal complexes. In the framework of this study the synthesis of new metal complexes of sodium, magnesium, aluminium, iron (III) ruthenium (III) and osmium (III) with caffeic acid was performed. The spectroscopic properties of these compounds were studied by means of FT-IR, FT-Raman, UV-Vis, ^{1}H and ^{13}C NMR. The quantum-chemical calculations (at B3LYP/LAN L2DZ level) of caffeic acid and selected complexes were done. Moreover the antioxidant properties of synthesized complexes were studied in relation to selected stable radicals (method of reduction of DPPH and method of reduction of ABTS). On the basis of the differences in the number, intensity and locations of the bands from the IR, Raman, UV/Vis and NMR spectra of caffeic acid and its metal complexes the effect of metal cations on the electronic system of ligand was discussed. The geometry, theoretical spectra and electronic charge distribution were calculated by the use of Gaussian 09 programme. The geometric aromaticity indices (Aj – normalized function of the variance in bond lengths; BAC - bond alternation coefficient; HOMA – harmonic oscillator model of aromaticity and I_6 – Bird's index) were calculated and the changes in the aromaticity of caffeic acid and its complexes was discussed. This work was financially supported by National Science Centre, Poland, under the research project number 2014/13/B/NZ7/02-352.

Keywords : antioxidant properties, caffeic acid, metal complexes, spectroscopic methods
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