DIAGNOSTICS OF MINERAL WATERS BY MEANS OF RAMAN SPECTROSCOPY AND ARTIFICIAL NEURAL NETWORKS

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Determination of salt composition of mineral waters and control of technical and waste waters containing (in toxic quantities) salts of heavy metals, nitrates, nitrites, sulfates, sulfides etc. is an extremely urgent problem. For the solution of this problem one needs express non-contact methods of diagnostics of water with possibility of their realization in real-time mode.

For this purpose, in this work laser Raman spectroscopy was used. The fundamental possibility of using Raman spectroscopy for the diagnostics of water is caused by the high sensitivity of characteristics of spectral Raman bands to the type and concentration of the compounds dissolved in water (1). However, even the high sensitivity of Raman bands to dissolved ions cannot provide the solution of the multi-parametrical inverse problem of the identification of ions and the determination of concentrations of each ion in multi-component water solutions, for example, in mineral waters. To resolve this problem artificial neural networks were used. Neural networks have shown the high efficiency in the solution of similar problems for five-component water solutions of salts already (2).

In this paper the results of the determination of the type and concentration of dissolved ions in water with Raman spectroscopy and neural network algorithms are presented. Presence and concentration of complex cations and anions in water (such as как NH_4^+, CO_3^{2-}, NO_3^-, PO_3^{2-}, SO_4^{2-}) were determined using changes of their own Raman bands in the 300-2000 cm^{-1} region (Fig. 1).

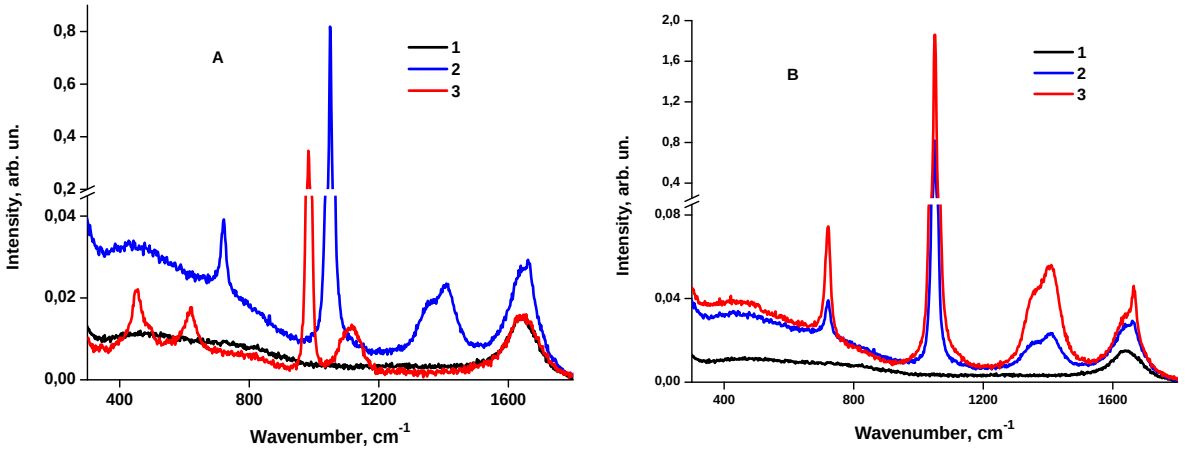

Figure 1: Raman spectra in the 300-1800 cm-1 spectral region for water and aqueous solutions of different inorganic salts (A): 1 –water, 2 - KNO_3 -1 M, 3 – Li_2SO_4 - 1M; and the salt KNO_3 of various concentrations (B): 1 –water, 2 - KNO_3 - 1 M, 3 – KNO_3 -3 M.

On the other hand, the presence in water of ions such as Na^+, K^+, Rb^+, Ca^{2+}, Cu^{2+}, Cl^-, I^-, Br^- etc. can be determined using their influence on the position and shape of the water Raman stretching band in the 2700 - 4000 cm^{-1} spectral region (Figure 2). Simultaneous use of both high-frequency and low-frequency regions of Raman spectra of water solutions (from 300 up to 4000 cm^{-1}) provides a possibility of complete characterization of the salt composition of mineral waters.

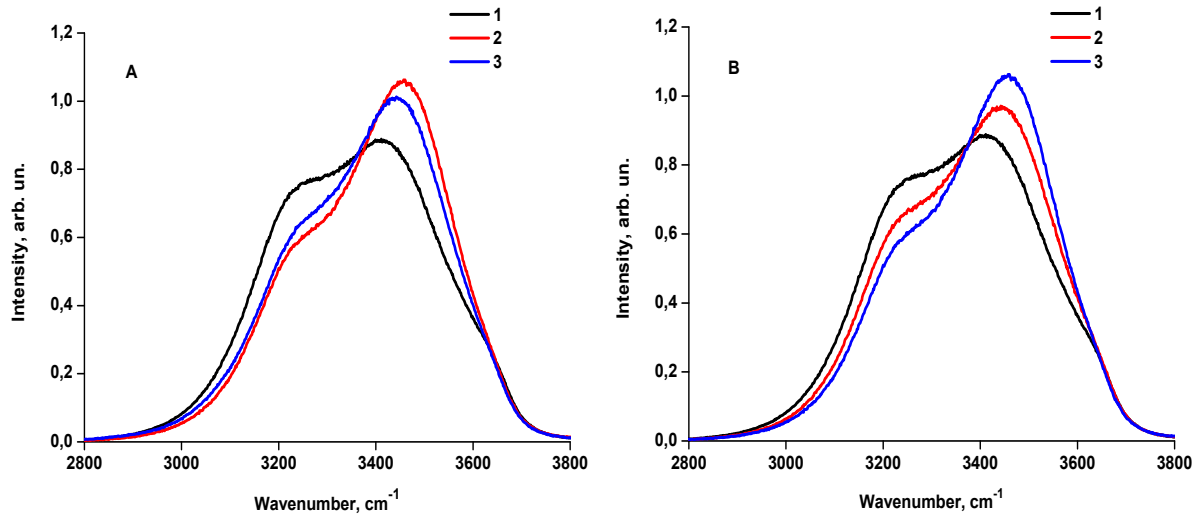

Figure 2: Raman stretching bands of water and aqueous solutions of different inorganic salts (A): 1- water, 2-CsI - 2M, 3 - NaCl, NH_4Br, Li_2SO_4 - 0.4 M, KNO_3 and CsI - 0.6 M; and of the salt CsI of various concentrations (B): 1- water, 2-CsI, 1M, 3- CsI, 2M.

A successful solution of such multi-parametrical inverse problem of laser Raman spectroscopy is provided by the application of artificial neural networks. “Experimental-based” approach (3) was used, optimal architecture and network parameters were found. The authors demonstrated that suggested method allows to determine a concentration of complex ions in water with accuracy 10^{-4} M, a concentration of simple ions with accuracy 10^{-3} M. The method was tested on natural mineral waters.

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