Integration of optical spectroscopy methods for determining the ionic composition of water using machine learning techniques

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Composition analysis of aqueous solutions is an important task in many fields of science and technology. To solve it, remote methods are required, enabling real-time operation. It is optical spectroscopy (OS) that offers remote capability and operational efficiency in this regard.

Inverse problems of OS in multicomponent liquid media, which cannot be solved with calibration curves with satisfactory accuracy, can be solved by neural networks (NN). This study attempts to establish the influence of simultaneous use of data from Raman scattering (RS), optical absorption (OA), and IR absorption (IR)of light by inorganic salt solutions on the solution quality of the inverse problem related to determining the concentrations of ions Zn^{2+}, Cu^{2+}, Li^{+}, Fe^{3+}, Ni^{2+}, NH_4^{+}, SO_4^{2-}, NO_3^{-}in water.

For this purpose, 3744 aqueous solutions with varying concentrations of salts $Zn(NO_3)_2$, $ZnSO_4$, $Cu(NO_3)_2$, $CuSO_4$, $LiNO_3$, $Fe(NO_3)_3$, $NiSO_4$, $Ni(NO_3)_2$, $(NH4)_2SO_4$, $NH_4(NO_3)$ were experimentally prepared, and their RS, IR, and OA spectra were obtained. The concentration of cations ranged from 0 to 1 M. Additionally, 16 RS and IR spectra of distilled water were recorded.

In this study, a comparative analysis of solution quality is conducted for the given inverse problem with NNs when RS and IR, RS and OA, IR and OA, RS, IR, and OA data are used simultaneously. For the most accurate determination of the concentration of each of the investigated cations, recommendations were developed for combining these spectroscopic methods.

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