Diagnostics of harmful impurities in aqueous media using spectroscopic methods and machine learning algorithms

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The results of the development of a method for diagnosing 8-component aqueous solutions containing lithium, ammonium, iron (III), nickel, copper and zinc cations, as well as sulfate and nitrate anions, by IR absorption spectra and optical density spectra using artificial neural networks are presented. The application of artificial neural networks to the obtained arrays of spectroscopic data made it possible to ensure the simultaneous determination of the studied ions in a multicomponent mixture with an accuracy that satisfies the needs of environmental monitoring of natural and waste waters, as well as diagnostics of technological environments.

Keywords: diagnostics of aqueous environments, spectroscopy, IR spectroscopy, absorption spectroscopy, machine learning methods, neural networks.

Introduction

The active development of industry and society is inextricably linked with an increase in environmental costs: losses of natural capital both at the initial stage of production (withdrawal of raw materials) and at subsequent stages (pollution by products of production). Disturbance of the qualitative and concentration balance of ions in the surface waters, waste waters and groundwater has a sharply negative impact on both human health and the ecological state of the environment as a whole. According to UN estimates, about 13% of the world's population live in conditions of constant freshwater deficit and after 20 years more than 6 bln people will suffer a shortage of freshwater [1]. According to the results of studies conducted by the Federal Service for Hydrometeorology and Environmental Monitoring (Roshydromet), which monitors environmental pollution and radiation conditions in the Russian Federation, in February 2022 alone, in 38 water bodies of the Russian Federation, 60 cases of extremely high surface water pollutions by substances of 1−4 hazard classes were recorded by the observation network [2]. As noted above, the main sources of pollution are enterprises of the metallurgical, mining, oil and pulp and paper industries, as well as housing maintenance and utilities. Thus, the pollution control of water resources is of critical nature. It is necessary to have the possibility of express diagnostics of various pollutants in water in order to quickly respond and correct the problem.

Thus, it is clear that the problem of water pollution is particularly relevant today. Modern methods make it possible to monitor the state of waters, but due to

the fact that in most cases the methods are contact and lengthy in implementation, it is impossible to ensure timely prevention of man-made disasters and their consequences. Optical monitoring methods provide fast and non-contact detection of pollutants, however, it is required to develop methods for the simultaneous determination of the type and concentration of many ions in multicomponent solutions, which can be implemented using machine learning methods (MLM).

At present, many different methods have been developed to determine the ionic composition of aqueous media. Basically, they can be divided into two types: contact and non-contact methods. Contact methods such as titration and chromatography are included in the GOST for the determination of various water pollutants. However, these methods are characterized by a long analysis time, the requirement for competent sample preparation, and the consumption of expensive reagents. It is clear that continuous monitoring of the state of aquatic media requires the development of remote methods, for example, spectroscopic methods. Spectroscopic methods make it possible to provide remote express monitoring of various pollutant components of aqueous media with minimal or no sample preparation.

The background for using optical methods to determine various impurities in aqueous media is that many pollutants have their intrinsic characteristic lines and bands in optical spectra. Thus, for example, in the optical absorption spectra of natural waters there are absorption bands of many heavy metal ions [3], the increased content of which in water is fraught with serious health problems [4]. At present, methods have been developed for determining the concentration of heavy metal ions from their optical absorption spectra [5].

However, despite clear successes, there are still a number of obstacles that prevent the use of these methods widely in practice. This is partly due to the fact that the optical density spectra of many substances overlap in a wide range of wavelengths, and it is often impossible to unambiguously distinguish the contributions of different impurities to a complex integrated spectral profile. On the other hand, not all pollutant ions have their intrinsic characteristic absorption bands, which makes it impossible to be limited by only one method for determining the composition of multicomponent mixtures.

Complex ions, such as nitrates, sulfates, and so on, have their intrinsic characteristic bands, and in vibrational spectra [6,7] the intensity of these bands is proportional to the concentration of the ions. Concentration of the corresponding ions in water can be determined on the basis of these ion's vibrational bands. Simple ions (for example, Cu, Ni, Pb) do not have their intrinsic characteristic vibrational bands, but their presence in solution can be determined by the deformation of the stretching vibration band of OH- groups of water molecules [8]. It is important to note that different ions have different effects on the shape of the stretching band of water [8]. Unfortunately, when studying a multicomponent solution, it is impossible to isolate the effect of each of the present ions on the stretching band of OH groups by traditional methods. This is due, on the one hand, to the fact that the deformation of the stretching band of water upon the addition of ions is of a weakly specific nature, and, on the other hand, to the inevitable interaction of ions not only with water molecules, but also with each other, which affects the shape of the spectrum as well.

In the last decades, similar multiparameter inverse problems of spectroscopy, i.e. identification of ions and determination of the concentration of each of them in multicomponent aqueous solutions from optical spectra, have been successfully solved using MLMs. The principal component analysis, the latent structure projection method, artificial neural networks (ANN), the method of support vectors and others are popular multivariate modeling techniques used for qualitative and quantitative spectral analysis. Recent advances in the field of machine learning demonstrate the ability of deep learning methods to detect complex structure in a large data set and extract important attributes, which in this scenario can be the type and concentration of a particular ion in a multicomponent solution [9]. Along with qualitative analysis (for example, the classification of cancer types based on IR absorption spectra of biological tissue [10]), the use of MLMs allows building of regression models for the quantitative analysis of samples. For example, the authors of [11] applied neural networks to Raman scattering spectroscopic data to successfully solve a three-parameter problem of determining the type and concentration of three nitrogenous bases in DNA: adenine, cytosine, and guanine. The obtained accuracies in determining the concentrations of nitrogenous bases in DNA were about 0.3 g/l, which is $1-2\%$ by weight of the number

of DNA molecules involved in biochemical reactions in molecular calculations.

This study presents the results of diagnostics of 8-component aqueous solutions containing cations of lithium, ammonium, iron (III), nickel, copper, and zinc, as well as sulfate- and nitrate- anions, by IR absorption spectra and optical density spectra using ANN. A method has been developed for identifying these pollutant ions in a multicomponent aqueous solution and determining the concentration of each of them.

Materials and methods

Subjects of the study

The subjects of the study were aqueous solutions of nitrates and sulfates: $Zn(NO_3)_2$ — 2.13 M, $ZnSO_4$ — 1.41 M, $Cu(NO_3)_2$ — 2.02 M, $CuSO_4$ — 1.16 M, $LiNO_3$ — 1.06 M, $Fe(NO_3)_3$ — 1.96 M, $NiSO_4$ — 2.21 M, $Ni(NO_3)_2$ — 1.40 M, $(NH_4)_2SO_4$ — 0.91 M, NH_4NO_3 — 0.82 M (by Baum-lux). Aqueous solutions of salts were prepared with the use of deionized water (Millipore Simplicity UV water purification system). The range of change in concentration of each of the salts in the solutions varied from 0 to 0.9 M, which corresponds, on average, to the range of change in the concentration of ions in the service waters of non-ferrous metal production plants (for example, in spent pickling solutions) [12]. For the application of ANN, 3744 salt solutions with various concentrations in deionized water were prepared. The simultaneous use of both sulfates and nitrates of the same cations made it possible to exclude the unambiguous determination of the cation concentration by analyzing the intrinsic vibrational band of the same anion.

Experimental methods

The prepared aqueous solutions of salts were studied by two independent methods: using optical absorption spectroscopy and IR absorption spectroscopy.

The optical absorption spectra were recorded using a Shimadzu UV-1800 double-beam spectrophotometer (Japan). A quartz cell (with an optical path length of 1.0 mm) with deionized water was placed in the reference channel. The measured sample was in a quartz cell with an optical path length of 1.0 mm Instrumental parameters for spectra recording are: range from 190 to 1100 nm with a step of 1 nm, fast scanning speed. The obtained spectra were not subjected to subsequent additional processing. The photometric accuracy of the instrument is ±0.004 of the optical density (with the optical density of 1.0), the photometric reproducibility is < 0.001 of the optical density (with the optical density of 1.0).

The IR absorption spectra were recorded using a Bruker Invenio R IR Fourier spectrometer equipped with a FTIR attachment with a diamond element. Instrumental parameters for spectra recording are: range from 400 to 4500 cm^{-1}, resolution of 4 cm^{-1}, averaging over 20 measurements. The obtained spectra were not subjected to subsequent additional processing. The photometric accuracy of the

instrument was at least 0.001 of the optical density (with the optical density of 1.0).

The application of ANNs

As it is already mentioned in the introduction, more and more often MMOs in general and ANNs in particular are used to solve inverse problems of spectroscopy. Three types of input data used to work with neural networks can be distinguished: 1) data obtained using a mathematical model of the process; 2) data obtained during a real experiment; 3) combination of data obtained both when using a mathematical model and during the experiment, i.e. the use of the quasi-model approach [13].

Each of these approaches has its own advantages and disadvantages. For example, when using the approach of „data from the model" the accuracy of solving the inverse problem using ANN is determined by the accuracy of the constructed mathematical model and the completeness of the description of processes. This approach has a clear advantage in that it is possible to form a large amount of input data, i.e. ensure the representativeness of the sets in a short time. However, the approach of „data from the model" does not take into account some possible processes and experimental noise. In the alternative approach of „data from the experiment" — when using the results of experiment as the initial data — all really occurring processes and noises are taken into account. However, the disadvantage of this approach is the high cost and labor intensity of conducting a large-scale physical experiment. The „quasi-model approach" consists in modeling the data using a certain number of experimental results, therefore it partially combines the advantages and disadvantages of both approaches mentioned above.

In this study, the approach of the „data from the experiment" was used, i.e., all the initial data (spectra of optical and IR absorption) used to train the ANN and to verify accuracy of the solution to the problem of determining the concentration of ions in aqueous solutions, were obtained during a physical experiment.

Results and discussion

The absorption spectroscopy

Fig. 1 shows IR absorption spectra of initial aqueous solutions of salts used in the course of the experiment to produce solution-mixtures of salts with pre-defined concentrations (specified in the *Subjects of the study* section).

As can be seen from the presented data, optical absorption spectra of aqueous solutions of the salts used have some features. Thus a peak in the region of 300 nm is observed in spectra of aqueous solutions of nitrates, which corresponds to the nitrate-anion absorption [14]. In the optical absorption spectra of aqueous solutions of sulfates and nitrates of nickel, absorption bands of nickel cations are observed in the wavelength ranges of 350−450, 530−850 and 900−1100 nm [15]. In the same manner, in the optical density spectra of aqueous solutions of copper salts, a
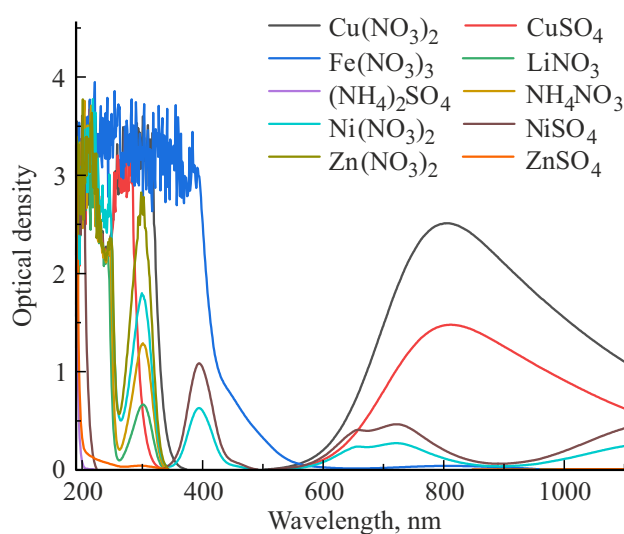

Figure 1. Optical density spectra of initial aqueous solutions of salts with the highest initial concentrations.

wide absorption peak of copper cations is observed with its maximum in the region of 802 nm [16]. The aqueous solution of ferrous nitrate is characterized by an intensive absorption of iron cations in the wavelength region of up to 600 nm [17]. In the obtained spectra of the optical density of aqueous solutions of the salts under study, the cations of zinc, lithium and ammonium do not have their characteristic bands.

As it is known, the dependences of absorption intensity of aqueous solutions of salts in a wide range of concentrations follow the Bouguer-Lambert-Beer law. However, when studying multicomponent salt solutions, the use of this law to determine the concentration of ions is complicated by the following. First, there are regions where optical density bands of different salts overlap in a wide wavelength range, which greatly complicates the determination of concentration of these salts in solutions from their optical density spectra. Second, a deviation from the Bouguer-Lambert-Beer law is possible due to the fact that the law itself assumes that the ability of a molecule to absorb light is not affected by other surrounding molecules in the solution [18]. Therefore, to solve the inverse multi-parameter problem of optical spectroscopy, i.e. to determine the concentration of each of the ions in multicomponent aqueous solutions, ANNs were used.

The IR-absorption spectroscopy

Fig. 2 shows IR absorption spectra of initial aqueous solutions of salts used in the course of experiment to produce solution-mixtures of salts with pre-defined concentrations (specified in the *Subjects of the study* section) and IR absorption spectra of aqueous solutions of copper nitrate with different concentrations.

As can be seen from the presented data, the IR absorption spectra of aqueous solutions of inorganic salts have some features. Intensive absorption bands of sulfate- and nitrate-
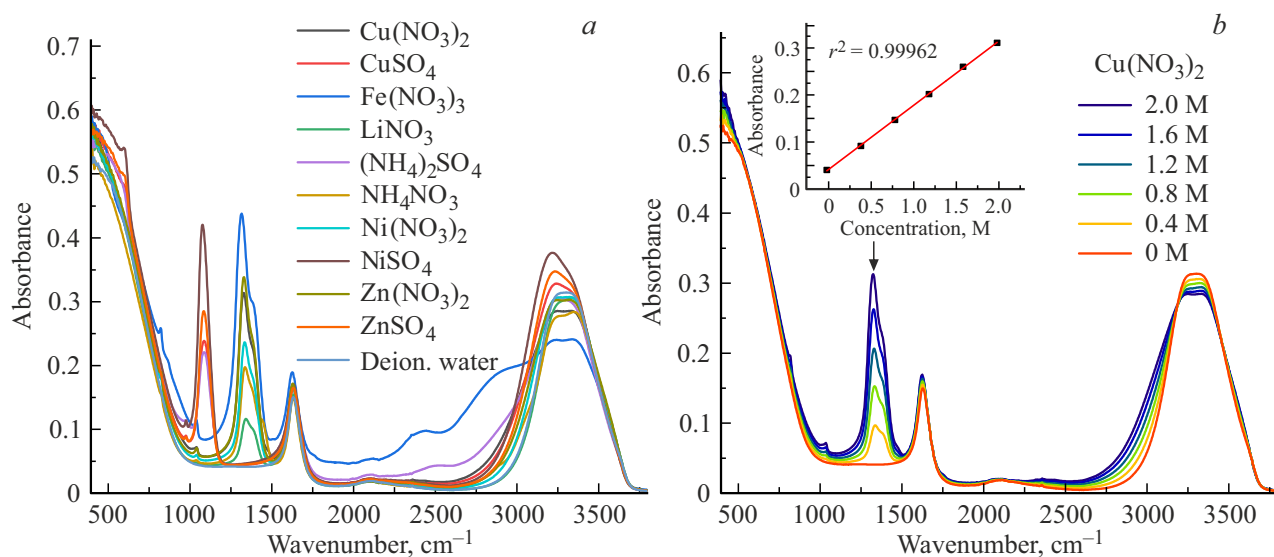
Figure 2. IR absorption spectra of the initial aqueous solutions of salts (*a*) and demonstration of the linearity of the IR absorption intensity dependence on the concentration by an example of the aqueous solution of copper nitrate (*b*).
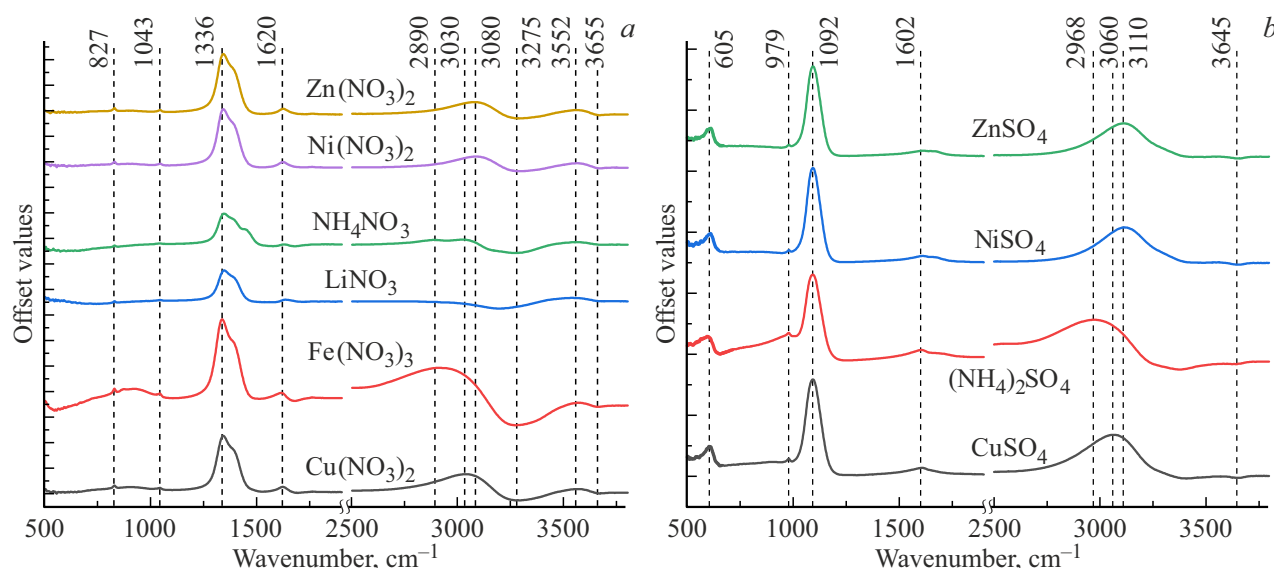

Figure 3. Difference spectra of aqueous solutions of nitrates and sulfates of the salts under study. Concentrations of aqueous solutions of salts are identical and equal to 0.8 M.

anions in the ranges of $996-1200$ and $1240-1491 \, \text{cm}^{-1}$ respectively. Simple ions, such as Zn^{2+}, Ni^{2+}, Cu^{2+}, etc., have no characteristic bands in the IR absorption spectrum, however, their content can be determined by the change in stretching vibration mode of OH-groups of water molecules [19,20]. To identify the most informative sections of the spectrum, difference spectra of aqueous solutions of the salts under study were built: the IR absorption spectrum of water was subtracted from IR absorption spectra of solutions (Fig. 3).

It can be seen from the presented data that in the spectra of aqueous solutions of nitrates of the studied salts in the region of „fingerprints" there are bands with maxima in

the vicinity of 827, 1043, 1336 and $1620 \, \text{cm}^{-1}$ due to vibrations of N-O groups in various configurations [21,22]. It is important to note that in the presence of different cations a displacement of some bands of nitrate-anions is observed. Thus, the most intensive band with a peak at $1336 \, \text{cm}^{-1}$ corresponding to $v3$-modes of N-O vibrations in the aqueous solution of iron nitrate is shifted relative to the same band in the aqueous solution of lithium nitrate by $8 \, \text{cm}^{-1}$ toward larger wavenumbers. This may be due to the fact that in the presence of various cations, nitrate anions are converted into various isomers that differ in their properties [22]. In the high-frequency region of difference spectra, a number of local extrema are observed in the

regions of 2890, 3030, 3080, 3275, 3552, and 3655 cm^{-1}. Such changes in the region of stretching bands of the IR absorption spectra of salt solutions compared with the bands of water indicate a different effect on the stretching bands of OH groups of various ions and a change in the strength of hydrogen bonds in water as a result of this effect [20,23]. It is the above changes in the characteristics of the vibrational bands of the spectra in multicomponent salt solutions due to the interaction of ions and water molecules, that are identification features for solving the problem of determining the type and concentration of ions dissolved in solutions using ANN [24,25].

From the point of view of solving the problem of identification and quantitative determination of pollutant ions, the detected changes in the spectra and their linear nature of change with respect to changes in concentrations (Fig. 2, *b*) make it possible to uniquely solve the one-parameter problem with a high accuracy. In a more complex problem, when working with multicomponent salt solutions, these changes in the spectra will be superimposed on each other, and, moreover, taking into account the sensitivity of the IR spectroscopy method, which makes it possible to determine various isomeric states of molecules (in particular, nitrates), the solving of the inverse problem of determining the concentration of pollutant in the solution will be hampered significantly.

The application of MLM

To solve the set inverse multiparameter problem, fully connected neural networks (NN), i.e. perceptrons with different numbers of hidden layers and neurons located in them, were applied in this study. This problem was solved in two versions: by optical absorption spectra and by IR absorption spectra of aqueous solutions of salts. For both options, three single-layer, two two-layer and one three-layer perceptron models were trained (the number of neurons in hidden layers is specified in brackets): (64), (128), (256), (128, 64), (256, 128), (256, 128, 64).

Intensities of the optical density and IR absorption spectra of prepared 3744 salt solutions were used in 911 channels (corresponding to the wavelength range from 190 to 1100 nm with a step of 1 nm) and in 1763 channels (corresponding to the range of wavenumbers from 400 to 3800 cm^{-1}), respectively. In each of the options, all obtained spectra of aqueous solutions of salts were randomly divided into 3 sets — training, validation and test — in the ratio of 70 : 20 : 10%, respectively. The first set was used to train the neural network — to adjust weight coefficients of neurons in the layers. The second set was used to prevent overfitting of the model and stop the network training in a timely manner. If during 500 training epochs the mean square error on the validation set did not decrease, then training was stopped and the network with the smallest error was selected. The test set was used to evaluate the quality of the solution to the inverse problem using independent data that was not previously used in the course of the NN training. To additionally prevent overfitting of the NN and eliminate the influence of the method of

The smallest MAE for determining the concentration of ions obtained as a result of the use of perceptrons with different architectures trained on the spectra of optical absorption and IR absorption of aqueous salt solutions

Cation/Anion	MAE, M (absorption)	MAE, M (IR absorption)
Zn	0.054 ± 0.004	0.029 ± 0.009
Cu	0.0083 ± 0.0007	0.031 ± 0.031
Li	0.092 ± 0.002	0.024 ± 0.024
Fe	0.017 ± 0.002	0.016 ± 0.016
Ni	0.012 ± 0.002	0.021 ± 0.021
NH$_4$	0.098 ± 0.015	0.027 ± 0.027
SO$_4$	0.049 ± 0.005	0.015 ± 0.015
NO$_3$	0.093 ± 0.003	0.038 ± 0.038

splitting the original data set on the problem solution, the cross-validation method was applied: the original array of spectra was randomly split 3 times. The results of applying the NN for three partitions were averaged. The neurons of the output layer of the NN determined the concentrations of 8 studied ions.

The Dropout method [26] was used as a network regularization method after each layer of neurons with a probability of neuron exclusion equal to 0.1. MSE (squared function) was used as the loss function. The search for the minimum of the loss function was carried out using the Adam algorithm [27]. The LeakyReLU function with a slope coefficient of 0.07 was chosen as the activation function.

To eliminate the influence of the initial initialization of the weights, 2 identical NNs were trained with different initial weights for each split of the cross-validation. The statistical indicators of problem solution for a given splitting were averaged over these two networks. As a result of application of NNs with different architectures, mean absolute errors (MAE) of determining the concentration of each ion were calculated. The results of ANN application are shown in Fig. 4.

As can be seen from the presented results, the accuracy of determining the concentration of ions does not strongly depend on the architecture of the NN, except for the applying a perceptron with one hidden layer and 128 neurons in it to the IR absorption data (Fig. 4, *b*). The best accuracies in determining the concentration from the optical absorption spectra of the studied ions are observed for copper, iron, and nickel cations, which have characteristic absorption bands. The table shows the smallest values of the MAE for determining the concentrations of each of the ions for each of the physical methods used, obtained as a result of applying various NN architectures.

It is not possible to unambiguously determine the best method for the simultaneous determination of the concentration of the studied ions. Thus, the MAE for determining zinc, lithium, iron, ammonium, sulfate, and nitrate ions from IR absorption spectra is less than the similar value determined from optical density spectra. On the other hand,
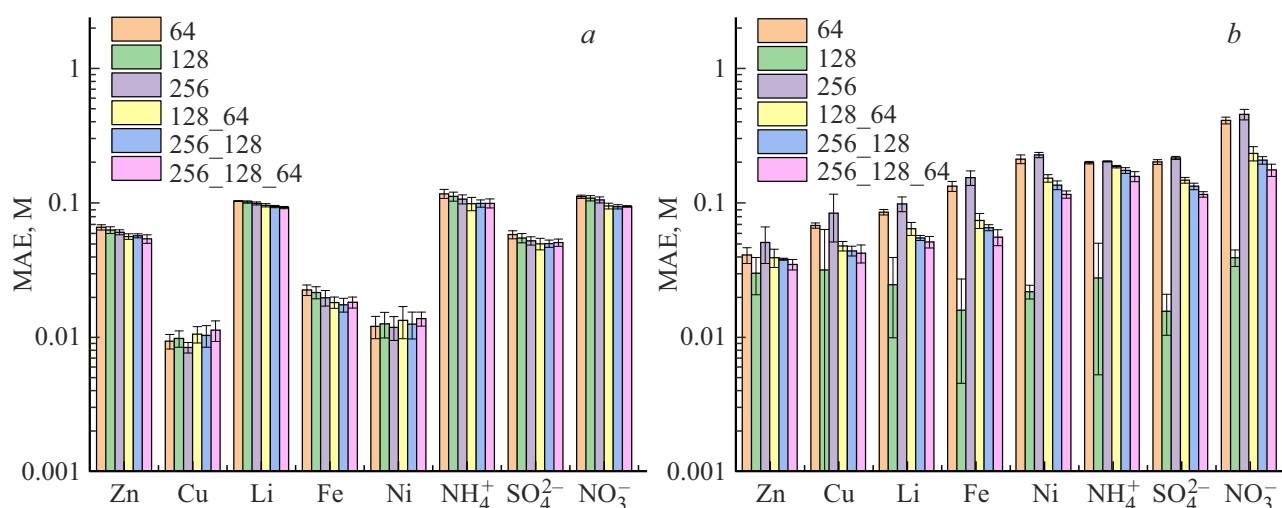
Figure 4. MAE diagrams obtained as a result of the use of NNs trained on the spectra of optical density (*a*) and IR absorption (*b*). Different colors correspond to different numbers of neurons (specified in the legend) in different hidden layers of perceptrons.

the MAE for determining copper and nickel ions from the optical density spectra is less than the MAE obtained with NN trained on the IR absorption spectra. Thus, to obtain the highest accuracy in the determination of different ions, it is necessary to use different NN architectures. Taking into account the currently available computation capacity, the use of several NNs will not increase the time spent on obtaining the result. It should be noted that in all cases the error in determining the MAE from the optical density spectra is less than the similar value obtained by training on the IR absorption spectra, which can be explained by the fact that the inverse problem being solved for the spectra of optical spectroscopy is described by a simpler mathematical model.

Conclusion

In this work, multicomponent aqueous solutions of inorganic salts containing $Zn(NO_3)_2$, $ZnSO_4$, $Cu(NO_3)_2$, $CuSO_4$, $LiNO_3$, $Fe(NO_3)_3$, $NiSO_4$, $Ni(NO_3)_2$, $(NH_4)_2SO_4$, NH_4NO_3 with concentration varied in the range from 0 to 0.9 M were studied using two spectroscopic methods, namely, the optical absorption spectroscopy and the IR spectroscopy. The application of artificial NNs to the obtained arrays of spectroscopic data made it possible to identify and simultaneously determine the concentration of each of the eight ions in a multicomponent mixture. The obtained accuracy in determining the concentration of the desired ions meets the needs of environmental monitoring of natural waters and waste waters, as well as diagnostics of technological media. Taking into account that commercially available instruments were used in the study, the developed method for determining the concentration of ions in process waters can already be used in production, which will directly contribute to environmental monitoring and health protection. The developed methodology has two directions

of further development: 1) improvement of the accuracy of solving the inverse problem and 2) increase in the ranges for determining the concentration, including for the qualitative and quantitative determination of the content of heavy metal ions in the human body.

Conflict of interest

The authors declare that they have no conflict of interest.

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