

Abstract

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Title of the diploma thesis: Development of multivariant spectrum analysis for heavy metal cations using dithizone

This experimental work deals with a basic study of multidimensional spectral analysis of heavy metal cations. Cobalt, nickel, lead, iron (ferric), zinc, cadmium, copper, and manganese cations were chosen as model analytes due to their general occurrence in drinking water and their potential toxicity to the human body at elevated concentrations. The metals were tested using the complexing agent dithizone (dissolved in isopropanol) in the range of pH 3 to pH 10 in a Lab-In-Syringe analytical system completed by an autosampler. A miniature spectrophotometer in combination with a halogen and deuterium light source and a 10 cm detection flow cell was used for spectrum registration. Extraction into an immiscible solvent, as typical for the analytical use of dithizone, was not done for speed and simplicity, i.e. avoiding additional parameters to be optimized. At the beginning of the work, spectra were measured in metal excess without the use of vacuum - the measurements showed high noise and lower resolution. This was resolved by creating a partial vacuum in the syringe pump system to aid solution degassing and by wrapping the detection cell with aluminium foil to reduce light transmission. Spectra were then measured in excess of dithizone applying these changes and sorted by the individual metals for one pH value as well as by the individual pH value for all metals. The spectra were compared to the spectrum of the unbonded dithizone. The results of the measurements at excess of dithizone showed that cadmium complexes formed even at the most acidic pH tested (pH 3) and only one absorption band is visible in the spectrum at 440 nm. For all other metals, complexation started between pH 4 and was completed at pH 8 with differences in spectrum. This proves that the reliability of a multivariant spectrum analysis method could be improved by spectrum acquisition not only at one but various pH values. Ferrous and manganese cations were considered as possible interferents in the work and had very similar spectra to dithizone itself, so that further studies using solvent extraction would be recommendable. For comparison of metal complexes at the same pH, it was shown that cadmium, zinc, and cobalt cations can be distinguished from each other.