

pH determination of small sample volumes using Raman spectra of azo dyes.

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A method enabling pH-value determination in the 1.4–13.9 range of several nanoliters of aqueous solutions was developed using Raman spectra of four azo dyes: azorubine, ponceau 4R, allura red and tartrazine. Based on pre-resonance Raman spectra of dye solutions in phosphate buffer and HCl/KOH solutions, partial least squares models allowing pH measurement in the given range with an error of less than 3% were developed and validated. Spectra of several dozen samples with known pH values were recorded for each dye. As the concentration of hydrogen ions increased, changes in the intensity, position and half-width of bands were observed. In all analyzed systems, the most pronounced differences between the spectra were observed at two extreme pH values. The changes occurred mainly within vibrational bands of the azo group and the carbonyl group and were related to their protonation/deprotonation, along with the change in the pH of the solution. The results of cluster analysis and DFT calculations suggest that in a strongly acidic environment, the studied dyes appear in the form of 2^- (azorubine, allura)/ 3^- (ponceau 4R, tartrazine) anions with a negative charge located within the SO_3^- groups and a protonated azo group. The alkaline environment leads to further deprotonation and formation of 3^- (azorubine, allura)/ 4^- (ponceau 4R, tartrazine) anions. Principal component analysis confirmed the coexistence of two distinct forms of dye molecules in the studied solutions.

Słowa kluczowe

pH determination, Raman spectroscopy, Azo dyes, PLS modeling, DFT calculations

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