Application of NIR SCAN class spectroscopy for express spectroscopic studies of objects with time-varying optical parameters.

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Near-Infrared (NIR) spectroscopy is a chemical analysis technique that uses the absorption of infrared radiation in the range of 800-2500 nm to determine the chemical composition of the sample under study. The analysis of NIR spectra allows for a fast and non-invasive determination of sample compositions in various fields, such as the food, pharmaceutical, medical, and agricultural industries. For a long time, there were some difficulties with the analysis of NIR spectra, which are not straightforward in interpretation. This was related to the lack of implementation of suitable analysis methods, which required adequate computational power. Today, a whole range of spectral analysis methods is known, appropriate programs exist, and the computational power of today's computers allows for the extraction of useful information from NIR spectra within a few seconds. One of the modern methods of NIR spectral analysis that can be applied is Artificial Neural Networks (ANNs) - mathematical models enabling machine learning. Their application in NIR spectral analysis allows for the automatic recognition of characteristic patterns and the detection of chemical compounds in samples. This method is particularly useful in the case of complicated, multi-dimensional NIR spectra, which are difficult to analyze using traditional statistical methods.

The second aspect of the work related to spectroscopy is the use of a compact, mobile DLP NIR Scan Nano EVM spectrometer, which can be ready for operation within a few seconds. The device records the spectrum in 2 seconds. It works in conjunction with a computer equipped with suitable software, generating files in .csv and .dat format, which can be easily implemented into other programs such as Matlab.

The study investigated objects that show spectral changes within a specific time range. Three groups of materials can be distinguished. The first group consisted of organic materials. Changes occurring in products related to maturation processes were studied, and in the case of green plants, changes occurring in leaves due to drying were investigated. This was a group of test objects that allowed for the development of a concept of working with NIR spectra in the Matlab program. The second group consisted of materials that can be used in electronics as adhesives or hermetization, where the curing process was studied. The target group consisted of PM (Perovskite Materials) used in the construction of modern photovoltaic cells, obtained through cooperation with the SAULE company. Spectral changes occurring in the materials over a period of 30 days were studied, with certain changes observed. Research on the improvement in stability of PSC (Perovskite Solar Cells) continues to be very intense as this is the main issue with modern cells.

Using the Matlab program, an appropriate ANN model was developed, which was trained and tested on the obtained base of perovskite materials spectra. Based on the MSE (Mean Square Error) analysis, the best learning methods and the optimal number of neurons in the hidden layer were selected. The impact of IDP (Initial Data Preprocessing) on the operation of the ANN was also determined. The program created by the author of this work allows for the recognition of the measurement time of a random spectrum from the measurement series and determines the measure of similarity of the selected spectrum to the others. Linking spectral changes with cell efficiency information could be a powerful tool for recognizing the stage of cell degradation.