

## Computer Analysis of ATR-FTIR Spectra of Paint Samples for Forensic purposes

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Infrared spectrometry is the method commonly applied to analytical examination of different materials for forensic purposes [1]. The advantage of this method is its non-destructive character as well as the possibility of identifying the main functional groups and structural elements of samples examined. However, IR investigations of such physical evidences as paint samples (microchips, smears on fabric), inks (on documents) and fibres are especially difficult. The reason is that the samples are often very small and, in addition, it is not usually possible to separate them entirely from the base.

An analytical tool offering quite unusually the possibility to examine the criminalistic traces without their prior separation from base is Attenuated Total Reflectance Fourier Transform Infrared (ATR-FTIR) technique. However, in case of ATR analysis of paints coats the influence of the base is usually significant hence the bands of not only a paint but also of the base are present in the reflection spectra. As a consequence, identification of the paint is very difficult or even impossible in practice. Therefore, this study was aimed to develop a mathematical approach allowing the undesired bands to be effectively eliminated from the paint spectra.

The Method of Subtraction and Normalization of IR Spectra (MSN-IR) was developed and successfully applied to extract the pure paint spectrum from the spectrum of paint coat on different bases acquired by the ATR-FTIR technique. The examined spectra (pure base and sample spectrum) were normalized in an iterative manner by the division by every each point of the calculated spectra. Number of obtained normalized spectra was equal with number of original spectrum points. Then, every normalized pure base spectrum were subtracted from every spectrum of the paint on foil (fabric). The subtractive results and the standard (pure paint) spectra were also normalized and after repeated process of comparison the final spectrum with the highest 'similarity' to the standard spectrum was found. The best subtraction was obtained when the value of correlation factor endeavored to zero.

The utility of the MSN-IR has been confirmed by analyses of several different paints sprayed on plastic (polyester) foil and fabric materials (cotton). A few examples of paint spectra obtained by the computer calculation were compared with those acquired from pure paints. It was found that proposed numerical algorithm allowed – in contrast to other mathematical approaches conventionally used for this aim – a pure paint IR spectrum to be effectively extracted without a loss of chemical information provided. Moreover, this approach is able to reduce the time consumption and to improve the reproducibility of spectral subtraction. The results obtained prove that the proposed procedure is a useful tool which could be applied in forensic discrimination and group identification of paints.

[1] J. Zięba-Palus, J. Mol. Struct. 511/512 (1999) 327–335.