

*Step by Step Filter:
an original approach for obtainment of highly informative derivative
spectra*

It is well known that the derivative spectroscopy provides possibilities for interpretation of absorption spectra, analysis of overlapping bands and quantitative analysis. These applications result from the fact that the derivative spectra can be easily obtained, being at the same time easy for interpretation and relatively simple as shape (both as consequence of the low noise level in the absorption UV-Vis spectra). The modern spectrophotometers as a rule have modules for calculation of the derivative curves in their operation software. However, it has been proved mathematically that the instrumentally derivatives attenuate in the long wavelength region. Therefore the approach called "Step-By-Step-Filter" (SBSF), allowing to obtain highly informative derivative derivatives with

substantial noise reduction and minimal curve distortion, directly from the measured absorption spectra, is suggested.

The derivatives calculated according to SBSF provide clear advantages in comparison with the instrumentally obtained: lack of attenuation in the long wavelength region and increased informativity; substantial noise reduction with minimal filter window; significant suppression of the computational noise; and they can be easily implemented in the software and hardware of the UV-VIS-NIR absorption, emission and CD spectrometers.

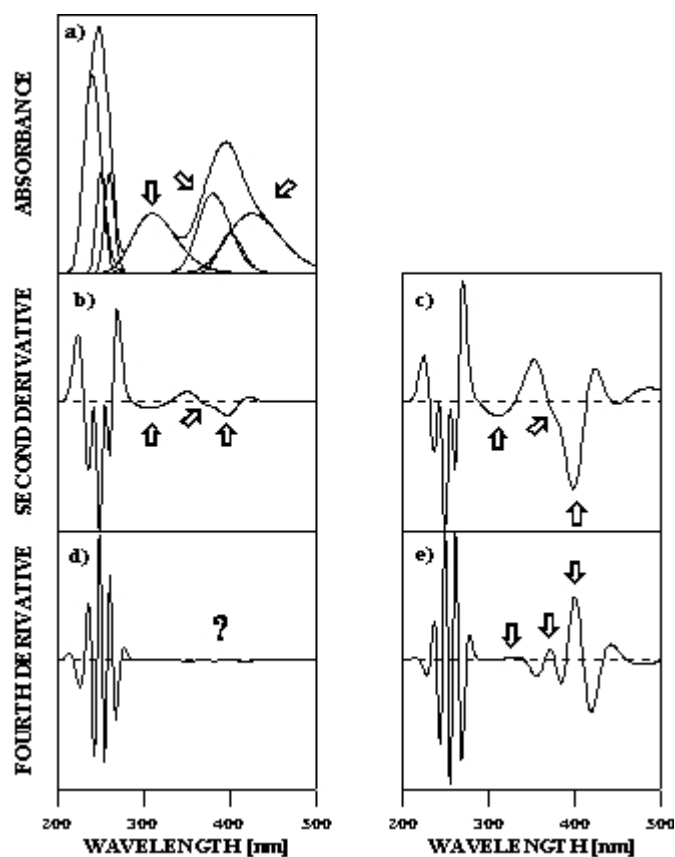


Fig. 1. a) Absorption spectrum with its composing individual bands; b) Instrumentally obtained second derivative; c) Second derivative obtained by SBSF; d) Instrumentally obtained fourth derivative; e) Fourth derivative obtained by SBSF.

General Description of The Method:

DRAWBACKS OF THE PRESENT STANDARDS FOR PROCESSING ABSORPTION SPECTRA RECORDED LINEARLY AS A FUNCTION OF WAVELENGTH.

L.Antonov;

Trends in Analytical Chemistry, 16(9), 536-543 (1997)

Theory and applications:

APPROACH FOR INCREASED INFORMATION FROM THE SECOND-DERIVATIVE SPECTRA IN UV-VIS ABSORPTION SPECTROSCOPY.

L.Antonov & St.Stoyanov;

Applied Spectroscopy, 47(10), 1712-1715 (1993)

NOISE REDUCTION IN SECOND DERIVATIVE UV-VIS SPECTROSCOPY.

L.Antonov & St.Stoyanov;

Spectroscopy Letters, 29(2), 231-239 (1996); 29, 967 (1996)

STEP BY STEP FILTER - AN APPROACH FOR NOISE REDUCTION IN THE DERIVATIVE UV- VIS SPECTRA.

L.Antonov & St.Stoyanov;

Analytica Chimica Acta, 324(1), 77-83 (1996)

FOURTH DERIVATIVE SPECTROSCOPY - A CRITICAL VIEW.

L.Antonov;

Analytica Chimica Acta, 349(3), 295-301 (1997)

Software description:

STEP BY STEP FILTER BASED PROGRAM FOR CALCULATIONS OF HIGHLY INFORMATIVE DERIVATIVE CURVES.

V.Petrov, L.Antonov, H.Ehara & N.Harada

Computers & Chemistry, 24(5), 561-569 (2000)