PHOTOELECTRON SPECTRA ANALYSIS OF SMALL ESTERS

Report on the visit

REFERENCE: Short Term Scientific Mission, COST CM0601
Beneficiary: Dr Malgorzata Smialek-Telega, Gdansk University of Technology
Host: Marie-Jeanne Hubin-Franskin, Université de Liège
Period: from 6/06/2010 to 12/06/2010 Place: Liège (BE)
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The main scope of the visit to the University of Liege, Belgium, (kindly supported by the COST CM0601 action) was for the beneficent to learn how to obtain, process and analyse photoelectron spectra of volatile organic compounds (VOC) on the example of small, simple esters.

During the visit it was possible to perform measurements and obtain photoelectron spectrum for ethyl formate. In addition, photoelectron spectra of three other molecules, isobutyl acetate, methyl acetate and ethyl acetate were processed and analysed. The spectra are shown in (Figure 1). The beneficent got familiar with a program dedicated to data analysis, Igor Pro.

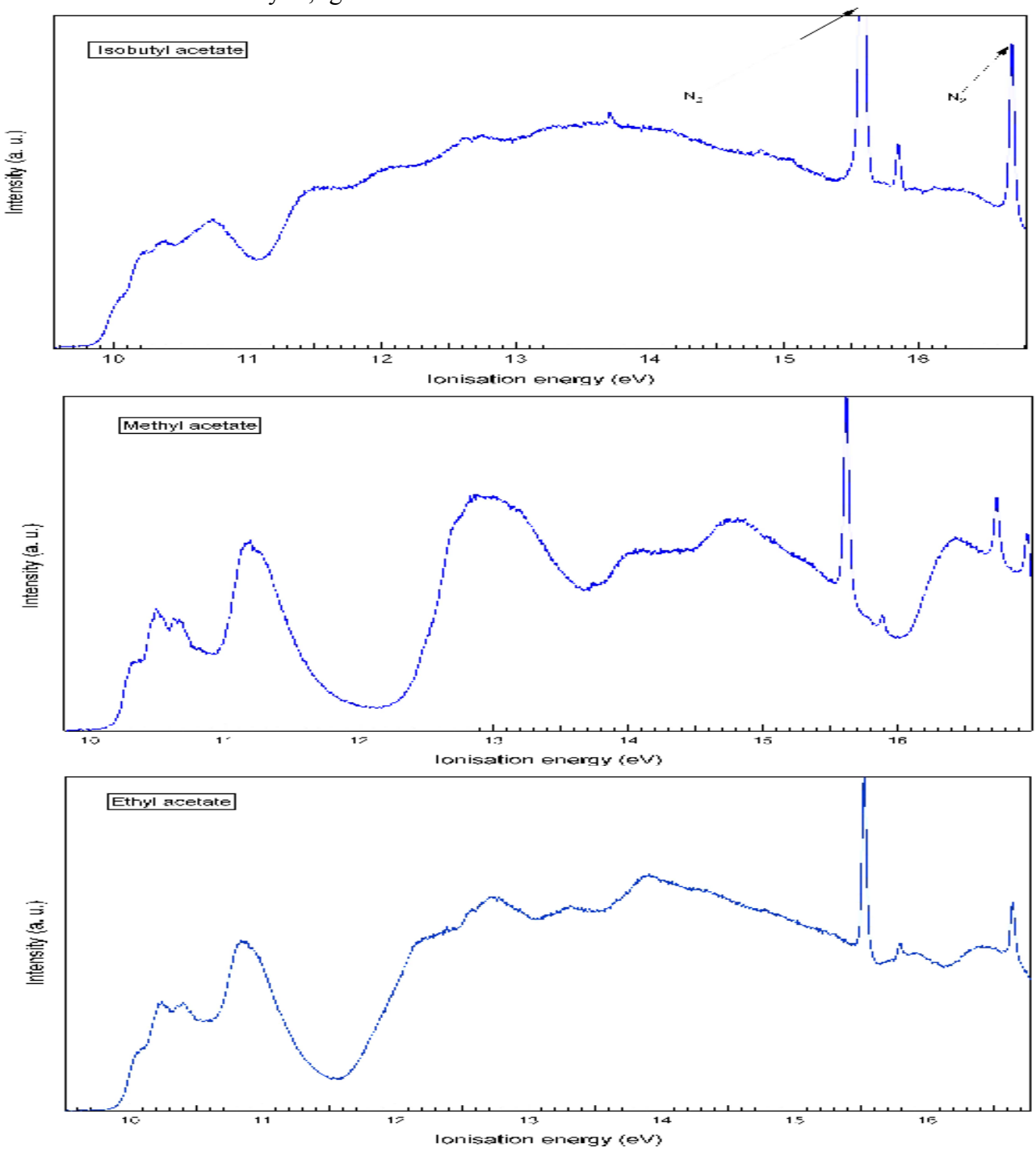

Figure 1 Photoelectron spectra of isobutyl acetate, methyl acetate and ethyl acetate.

From the obtained data it was possible to assign the ionisation energies for the molecules of interest using Voigt functions. Sample assignment of ionisation energies for first and second electronic band of methyl acetate is shown in Figure 4.

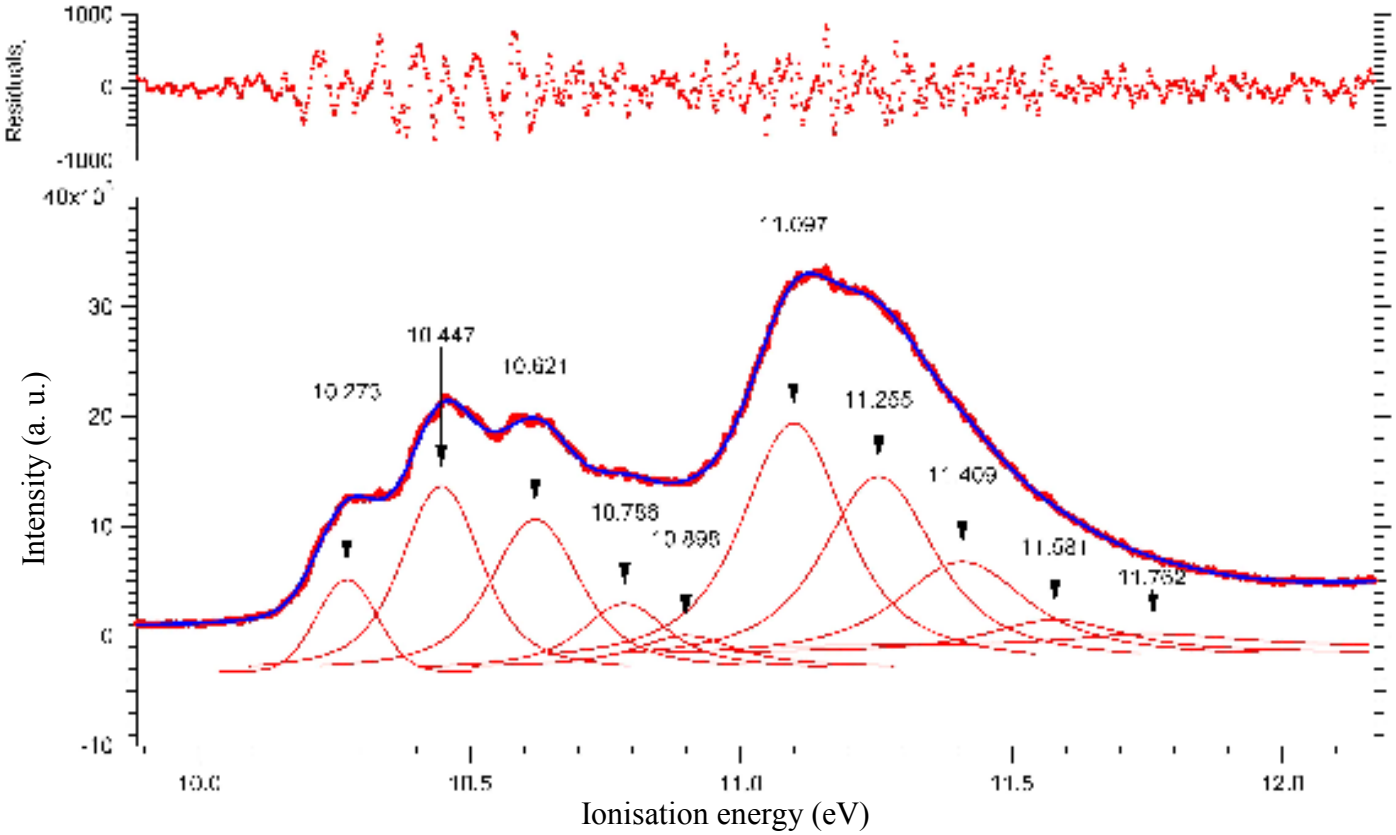

Figure 2 Voigt function fit and ionisation energies assignment for methyl acetate.

The data processed and analysed during this visit will be useful in analysing VUV-UV absorption spectra of esters that were already collected at University of Aarhus, Denmark and should result in a publication in international journal.