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Valence and ionic lowest-lying electronic states of small esters studied by high resolution vacuum ultraviolet photoabsorption, photoelectron spectroscopy and *ab initio* calculations

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Esters are an important class of oxygenated volatile organic compounds used in food flavorings, perfumes and other cosmetic products. They are present in fruits and pheromones and are emitted to the atmosphere naturally. Esters are also formed in the atmosphere as a product of the oxidation of ethers. Some of them form poly-molecule chains and are used in plastics. Phosphoesters form DNA backbone, while nitroesters are known for their explosive character. Some small ester molecules were reported to be found in the interstellar space. It was also shown that esters may be a product of hydroxyl radical-initiated oxidation of various ethers in troposphere.

Although esters are not very toxic, their degradation in the atmosphere may lead to production of more toxic and reactive species.

In our present study we have focused on smaller monoesters. The main purpose of our work is to understand, how the carboxylic and alcohol group distribution within the molecules influences their physical properties and reactivity.

In this communication we would like to present our findings for ethyl formate [1], isobutyl formate (Figure 1) [2] and ethyl acetate [3], studied experimentally as well as theoretically. The high-resolution VUV photoabsorption spectra shown here were measured at the UV1 beam line, using the ASTRID synchrotron facility in Aarhus University, Denmark. The photoelectron spectra of esters were measured either at the VLS-PGM beamline at the Canadian Light Source facility in Saskatoon, Canada, using a Double Toroidal Coincidence Spectrometer or at the Université de Liège, Belgium, using the He(I) radiation.

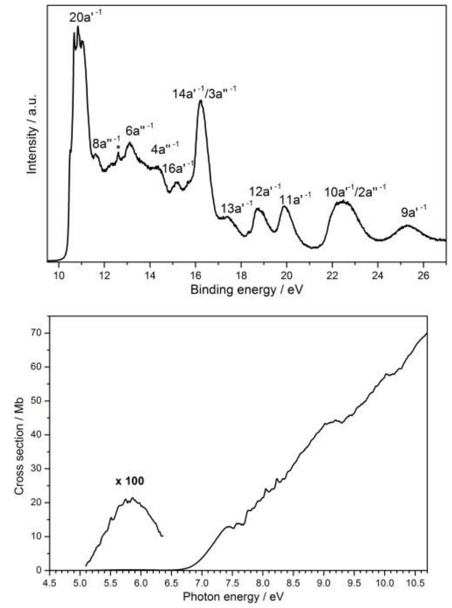

Figure 1. Photoelectron (upper) and photoabsorption (lower) spectrum of isobutyl formate, $C_5H_{10}O_2$.

The results presented here are supported by *ab initio* calculations in order to allow for correct assignment of all vertical and adiabatic ionization energies resolved in the spectrum as well as proper assignment of valence states and Rydberg transitions found in the photoabsorption spectrum.

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