Ionization yield and fluorescence excitation functions in the resonant C1s electron excitation of terpenes and terpenoid molecules

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To provide insight in the electronic behavior of chiral molecules in a chiral environment the total ionization yield and fluorescence excitation functions of different terpenes and terpenoid molecules were measured after photon excitation.

The experimental data were obtained using the PIFS technique (Photon Induced Fluorescence Spectroscopy) [1]. Chiral molecules in a heatable target cell were excited by circular polarized synchrotron radiation provided by the P04 beamline at PETRA III. The excitation energy was varied in the C1s excitation region with a stepwidth of 100 meV with a bandwidth of 200 meV and was calibrated to resonances of CO_2 [2].

Fluorescence photons ranging from 280 nm to 680 nm were measured and integrated for each energy step, resulting in the total fluorescence excitation functions of the given spectral range. A voltage of +10 V was applied to one of the insulatedly mounted target cell apertures to measure the total ion yield. These measurements were compared to resonant absorption spectra TD-DFT calculations based on the PC-3 basis sets [3,4] and B3LYP exchange functional [5]. The resonance energies for the 40 lowest orbitals were calculated for each carbon atom and convoluted with a Voigt profile (σ_{Gauss}=0.20 eV $\sigma_{Lorentz}$=0.12 eV).

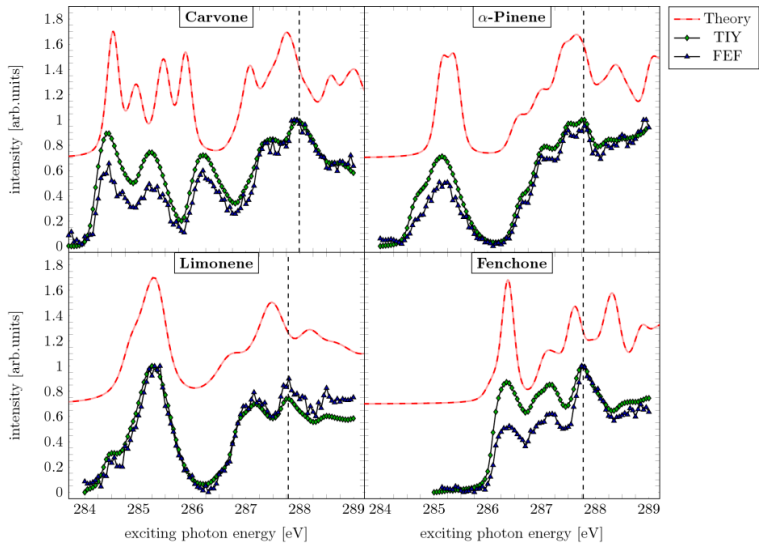

Figure 1: Comparison of the measured total ion yield (TIY, green diamonds), fluorescence excitation function (FEF, blue triangles) and Theory (red curve). All curves are normalized to their particular maximum and the theoretical curves were shifted in their absolute values for clearness. The dashed line indicates a possible excitation of a stereo center electron. Here, future investigations on chirality should be focused.

The measured energy dependency of the total ion yields, fluorescence excitation functions and the corresponding theoretical curves are shown in Fig. 1. A qualitative and an overall quantitative agreement were achieved. Therefore, the different features can be addressed to resonances of the different carbon core shell electrons.

References

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