

# Investigation of the absorption structure of K-shell excited terpenes and their subsequent fragment fluorescence decay

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Relative ionization cross sections, fluorescence excitation function and dispersed fragment fluorescence spectra of limonene, carvone, fenchone and  $\alpha$ -pinene were recorded after resonant excitation of C1s resonances from 283 – 289 eV by photoabsorption of synchrotron radiation. The fluorescence spectra are shown in the spectral region from 385 nm to 495 nm. Resonance like structures were observed in the relative ionization cross sections.

Commonly, chirality is investigated by the response of the molecule on the interaction with polarized probes, particularly with circularly polarized light, looking for dichroic effects. Until now fluorescence emission after an inner shell excitation step was not used as a probe for chirality. A potential dichroism in fluorescence emission may be observed after an inner shell resonant excitation to a delocalized orbital, its subsequent relaxation by fluorescence emission, or its dissociation taking the chiral information to the angular distribution of excited fragments or to the emission of fragment fluorescence. However, there is essentially no information about the excitation energies and decay routes of inner shell resonances even of prototypical chiral molecular systems.

Therefore, the poster presents first results of investigations of C1s resonant excitations of four prototypical chiral molecules: limonene, carvone, fenchone and  $\alpha$ -pinene. The main aim was to determine resonance excitation energies and relative ionization and fluorescence emission cross sections as a first step towards understanding their decay pathways. Additionally dispersed fluorescence emissions spectra in the visible spectral range have been recorded (see Fig. 1).

Time dependent density functional theory (TD-DFT) calculations were performed to reproduce the observed resonance-structures of the investigated molecules.

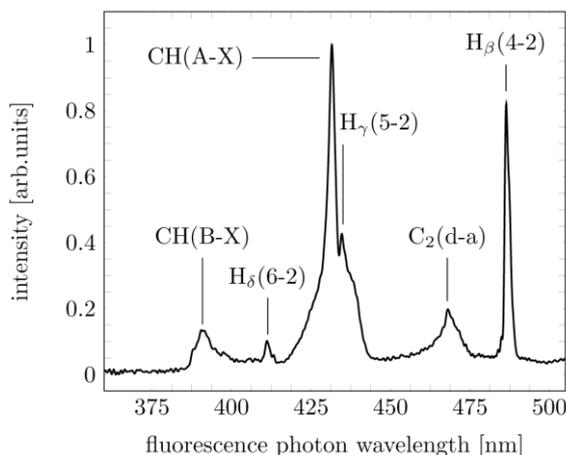


Fig. 1: Exemplary dispersed fluorescence for fluorescence wavelengths between 385 nm and 495 nm. Peaks were assigned according to [1] and [2].

## References:

- [1] Ye, C., Suto, M., Lee, L.C., J. Chem. Phys., **89**, 2797 (1988).
- [2] Han, J.C., Ye, C., Suto, M., Lee, L.C., J. Chem. Phys., **90**, 4000 (1989)