

# Investigation of site selectivity in the fragmentation of core-excited 1,3-butadiene near the central and terminal carbon K edges

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Site selectivity is well known in the electronic decay of core-excited states in molecules and adsorbate systems. An early study by Hayes and Eberhart reported that the population of different final states for C1s or S 2p ionization in thiophene was reflected in the fragmentation pattern [1]. Site-selective Auger decay is documented in molecules such as nitrous oxide [2] where tunable synchrotron radiation is used for resonant excitation of core-shell electrons localized at different atomic sites in the molecule [3], this does not always correlate to specific fragmentation channels some cases exhibit strong site-selective fragmentation after core-electron ionization [4]. A promising system for site-selective studies is the 1,3 trans butadiene molecule since the chemically-shifted central and terminal carbon 1s- $\pi^*$  resonant excitation is easily resolvable in the absorption spectrum [5]. Site-selective Auger decay was found for the participator decay using high-resolution electron spectroscopy confirming the existence of localized electronic decay channels [6].

The aim of this work is to investigate whether the final dicationic states that are populated after resonant excitation retain the memory of the initial core-excited state. To this aim the dissociation of core excited 1,3-butadiene at the C1s edge has been studied by a multiple-ion coincidence momentum imaging spectrometer [7] at the soft x-ray beamline I411 on the MAX-II located in MAX-Lab, Lund, Sweden. The coincidence maps show that after a first bond break of the carbon backbone to produce the asymmetric cation pair  $C_3H_3^+/CH_3^+$  and the symmetric pair  $C_2H_3^+/C_2H_3^+$  leads these dissociate producing numerous secondary fragments. While specific fragments are not identified in the double-coincidence spectra differences in the overall ionization state and intensity are measured.

Possible reasons for the lack of selectivity are discussed. These include the delocalized nature of the final states populated after C-VV Auger decay and the loss of information via cascade processes that result in a plethora of small fragments. Another important mechanism is the energy conversion between electronic states and vibrational states that has been reported for other molecules [8].

## References:

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