

# Dynamical (e,2e) results on biomass fragments and biomolecules

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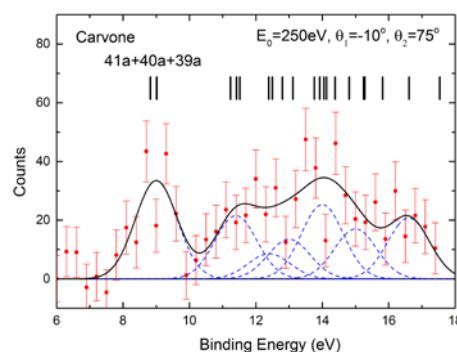
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**Synopsis** We report on joint experimental and theoretical studies of the kinematically complete electron impact ionization of molecules that represent key subunits of biomolecular systems.

Detailed knowledge regarding the dynamics of electron-impact ionization of large molecules is important in describing charged-particle transport through biomaterials, and how it can facilitate electron driven chemical changes within that material. Developing a fundamental understanding of how the geometric and electronic structures of the molecules found within biomolecular systems influence the scattering phenomena is important in realizing innovations in electron beam or plasma biomaterial processing and radiation interactions with living systems.

To assist in these efforts, we have performed a series of electron impact ionization experiments on large molecules that are frequently found within important biomolecular systems. Here we have measured triple differential cross sections (TDCSs) for the electron impact ionization of a target molecule under coplanar asymmetric energy sharing kinematic conditions. These measurements are performed using an (e,2e) coincidence technique on an apparatus that has been described previously [1]. Our setup is configured for measuring angular distributions of the TDCSs for a slow (20 eV) ejected electron, when the outermost molecular orbitals of the target molecule is ionized by an intermediate energy electron (250 eV). These angular distributions are observed for a combination of fixed scattered electron angles.

Our experimental investigations are supplemented by theoretical calculations of the TDCS for the ionization processes under the experimental kinematical conditions. Here the theoretical calculations are performed at the molecular 3-body distorted wave level [2]. Through a comparison of theoretical and experimental data, we can begin to assess the validity of approximations employed within the calculations.



**Figure 1.** A preliminary (e,2e) binding energy spectrum for R-carvone.

Here we will present some of our recent results for the electron impact ionization of R-carvone (see Figure 1), a naturally occurring bioactive monoterpene. We will also summarize some results from our recent investigation on parbenzoquinone [3], which is the prototypical subunit for quinones that are found in the electron transport chain of photosynthesis and respiration. Results for other large molecules that represent key constituents of biomass [4,5] will also be discussed.

## References

- [1] S. J. Cavanagh and B. Lohmann 1999, *J. Phys. B: At., Mol. Opt. Phys.* **32**, L261.
- [2] D. H. Madison and O. Al-Hagan 2010, *J. At., Mol., Opt. Phys.* **2010**, 367180.
- [3] D. B. Jones *et al* 2016, *J. Chem. Phys.* **145**, 164306.
- [4] D. B. Jones *et al* 2015, *J. Chem. Phys.* **143**, 184310.
- [5] G. B. da Silva *et al* 2014, *J. Chem. Phys.* **141**, 124307.

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