

The electron-furfural scattering dynamics for 63 energetically open electronic states

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Synopsis We report on integral-, momentum transfer- and differential cross sections for elastic and electronically inelastic electron collisions with furfural ($C_5H_4O_2$). The calculations were performed with two different theoretical methodologies, the Schwinger multichannel method with pseudopotentials (SMCPP) and the independent atom method with screening corrected additivity rule (IAM-SCAR) that now incorporates a further interference (I) term.

Over the past three decades the interest in developing new and/or improved technologies, notably for lignocellulosic biomass conversion to biofuels and other biomaterials, has been boosted by a scenario in which the growing worldwide demand for energy must be met while addressing concerns about global climate changes. Among the challenges to be overcome, the natural resilience of plant cell walls, in particular to the destructive action of microbial and enzymatic processes, is nowadays recognized as being largely responsible for the high cost of lignocellulose conversion into biomaterials that possess a high added value. Aiming to address this question, theoretical and experimental investigations revealed that free-electrons and radical species formed within atmospheric-pressure plasmas have the ability to contribute to the deconstruction of biomass [1]. In this context, low-energy electrons produced within the plasma environment have the potential to induce breakage of chemical bonds through dissociative electron attachment, electron-impact excitation, and other fragmentation processes. In the present work, the SMCPP with N energetically open electronic states (N_{open}) at either the static-exchange ($N_{open}ch-SE$) or the static-exchange-plus-polarisation ($N_{open}ch-SEP$) approximation was employed to calculate the scattering amplitudes for electron collisions with furfural at impact energies lying between 5 eV and 50 eV, using

a channel coupling scheme that ranges from the 1ch-SEP up to the 63ch-SE level of approximation depending on the energy considered. For elastic scattering, we found very good overall agreement at higher energies among our SMCPP cross sections, our IAM-SCAR+I cross sections and the experimental data for furan (a molecule that differs from furfural only by the substitution of a hydrogen atom in furan with an aldehyde functional group). This is a good indication that our elastic cross sections are converged with respect to the multichannel coupling effect for most of the investigated intermediate energies. However, although the present application represents the most sophisticated calculation performed with the SMCPP method thus far, the inelastic cross sections, even for the low lying energy states, are still not completely converged for intermediate and higher energies.

References

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