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Dimerization effects on the e^--$(H_2CO)_2$ scattering cross sections

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Abstract: Electron-induced DNA damaging have been associated to subionization and subexcitation processes [1]. Hence, several studies on electron scattering with biological molecules have appeared in the literature in the recent past, however quite a few explored weakly bound systems [2,3]. Formaldehyde dimer $(H_2CO)_2$ present one of the simplest examples of systems containing a C-H...O interaction, that is often found in the structures of important biomolecules such as amino acids, sugars, DNA and RNA. Therefore, the system can serve as a prototype for investigations about the damage caused by low-energy electrons when interacting with larger biochemical units present in living tissue.

In this work we present a theoretical investigation on e^--$(H_2CO)_2$ scattering. Several cross sections of the two most stable structures reported by Dolgonos [4] (the Cs and the C_2h ones) were computed in the 1-50 eV energy range. For comparison purposes, all the cross sections of the monomeric system were also determined.

The EPolyScatD suite of codes (originally developed by Gianturco *et al.* [5] and modified by de Souza *et al.* [6]) was employed to perform all the scattering-related computations. In the referred package, a complex optical potential (COP) is used to represent the collision dynamics and a single-center expansion method combined with the Padé approximation is used to solve the scattering equations. The COP incorporated in EPolyScatD is given by:

$$V_{opt} = V_{st} + V_{ex} + V_{cp} + iV_{ab}\,.$$

In the above equation, V_{st} and V_{ex} are the static and the exchange components, respectively. V_{cp} is the correlation-polarization contribution obtained in the framework of the free-electron-gas model [7], and V_{ab} is the improved model absorption potential developed by our group [8].

In Fig. 1 we show our calculated results of the Momentum Transfer Cross Sections (MTCS).

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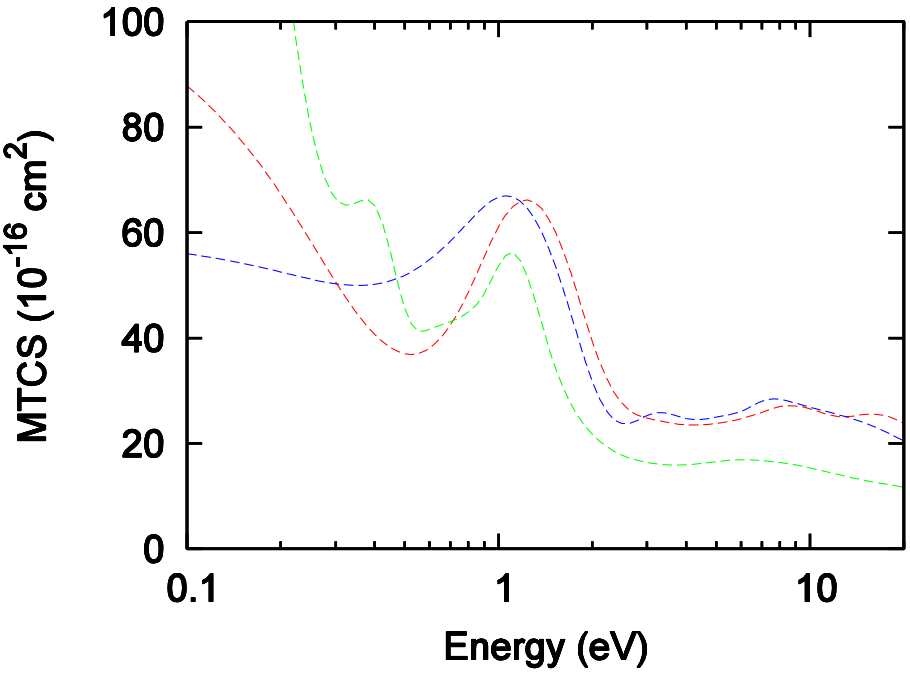

Figure 1. MTCS of the electron scattering. Green dashed curve, results of e^--formaldehyde monomer; red dashed curve, results of e^--(Cs dimer); blue dashed curve, results of e^--(C_2h dimer).

It is possible to notice the occurrence of a shape resonance (around 1.0 eV) in all three species. Interestingly, the feature seen in the Cs dimer presents a blue shift (about 0.3 eV) when compared to the monomer, while the C_2h dimer show the feature at the same energy (or slightly red shifted by 0.05 eV). Additional results will be presented at the Conference.

Key-words: Electron scattering, formaldehyde, cross sections
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