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

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Synopsis *We computed electron scattering cross sections for the two most stable structures of the formaldehyde dimer.*

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 for the two most stable structures reported by Dolgonos [4] (the Cs and the C_2h ones) were computed in the 1-25 eV energy range. For comparison purposes, all the cross sections of the monomeric system were also determined.

The EPolyScatD code (originally developed by Gianturco *et al.* [5] and modified by de Souza *et al.* [6]) was applied to solve the scattering equations. A complex optical potential, given by:

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

is used to represent the collisional dynamics. 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 momentum transfer cross sections (MTCS). 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.

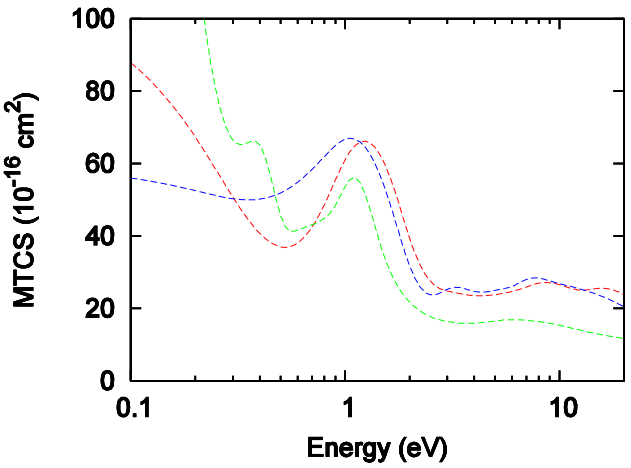

Figure 1. MTCS of electron scattering. Green dashed curve, results of e^--formaldehyde monomer; red dashed curve, results of e^--(Cs dimer); blue dashed curve, results of e^--(C_2h dimer).

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