Determination of energy-transfer distributions in ionizing ion-molecule collisions

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Synopsis The main objective of this study is to determine the energy transfer occuring in ion-molecule collisions. In order to solve this problem, we followed two approaches; the first one by validating a purely experimental method and the second one by testing a new theoretical model M_3C (Microcanonical Metropolis Monte Carlo).

Nowadays, several studies regarding medical applications on radiation damage are being carried out, in particular, concerning hadrontherapy where ions are used as ionizing particles. In order to better understand the fundamental processes causing these damages, such as ionization and fragmentation, it is necessary to study the system at the molecular level, thus in the gas phase. The comparison between theoretical models and experimental results requires the knowledge of the energy-transfer distribution during ion-molecule collisions. The aim of this study is to determine this energy distribution. We have chosen to investigate the furan molecule, a very reactive organic species, composed of an aromatic ring with five atoms including one oxygen atom. This molecule can be considered as a model or analogue of the nucleotides sugar, a part of the DNA [1]. In order to determine the energy-transfer distribution during the collision between an ion and a furan molecule, we have applied two approaches. The first one is purely experimental; the distribution is obtained by fitting ion collision mass spectra with a combination of all PEPICO (Photon-Electron Photon-Ion COincidence) spectra after photon interaction [2]. The second method relies on a new theoretical model: M_3C (Microcanonical Metropolis Monte Carlo) which provides fragmentation probabilities as a function of the excitation energy of the molecule [3]. Once again, the energy distribution is obtained by fitting ion collision mass spectra with the branching ratios obtained by this model. Figure 1 shows good agreement between the energy distribution of furan obtained by collisions of Ar^+ and Xe^{25+} ions compared with PEPICO data and M_3C calculations. The result is considered as an accurate prediction of the excitation energy distribution of complex molecular ions produced in collision with fast ions. It should be noted that this method does not require the knowledge of the initial and final states of the projectile nor the ionization potential of the target.

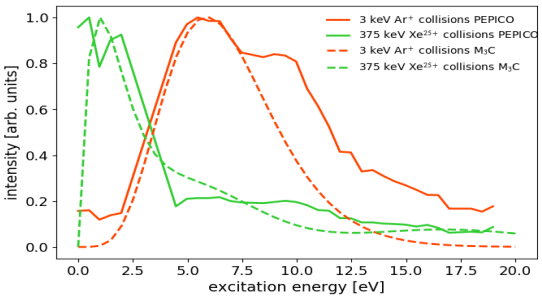

Figure 1. Distributions of the energy-transfer in collisions of Ar^+ and Xe^{25+} with the furan molecule obtained with the two approaches proposed here.

References

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