Journal of Physics: Conference Series

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XXIX International Conference on Photonic, Electronic, and Atomic Collisions (ICPEAC2015) IOP Publishing
Journal of Physics: Conference Series **635** (2015) 072060 doi:10.1088/1742-6596/635/7/072060

Theoretical Modeling of Mass Spectrometry

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Synopsis We present an implementation of the Microcanonical Metropolis Monte Carlo method based on statistical mechanics and electronic structure calculations. The method is designed to study any kind of fragmentation process. Here we show its capabilities to predict mass spectra of simple molecules.

When a highly energetic particle hits a neutral molecule, part of its energy is transferred to the molecule. If this energy exceeds the ionization energy, ejection of one electron occurs, which generates a molecular ion in an excited state. Then, the molecule breaks leading to a characteristic fragmentation pattern. As the excitation energy increases, the number of channels, abundance and variety of the ionized species also increase. The main hypothesis of our method is that the nature and extent of these reactions depend only on the ion's structure and its internal energy, irrespective of the ionization mechanism.

Under this hypothesis, the dynamical evolution of the many-body system is mainly guided by the accessible phase-space. Thus, statistical mechanics provides the appropriate theoretical framework to conduct this kind of simulations. In this context, we have developed the statistical Microcanonical Metropolis Monte Carlo (M_3C) method [1, 2], which is based on a specific random way to move in the phase-space until a region of maximum entropy is reached, where physical observables are computed by performing a statistical average. The minimum information that M_3C needs is the electronic energy, molecular geometry and vibrational frequencies for all possible molecules/fragments involved in the fragmentation process, and the main information provided is the breakup-curves (fragmentation probabilities as a function of the excitation energy). The mass spectrum is obtained by a weighted sum of these curves by using the internal energy distribution of the parent ion resulting from the process of electronic ionization.

In this contribution we will show some results for benchmark systems. In particular Fig. 1 shows the capabilities of M_3C to describe the fragmentation of the difluoromethane molecule (CH_2F_2) with their associated breakup-curves.

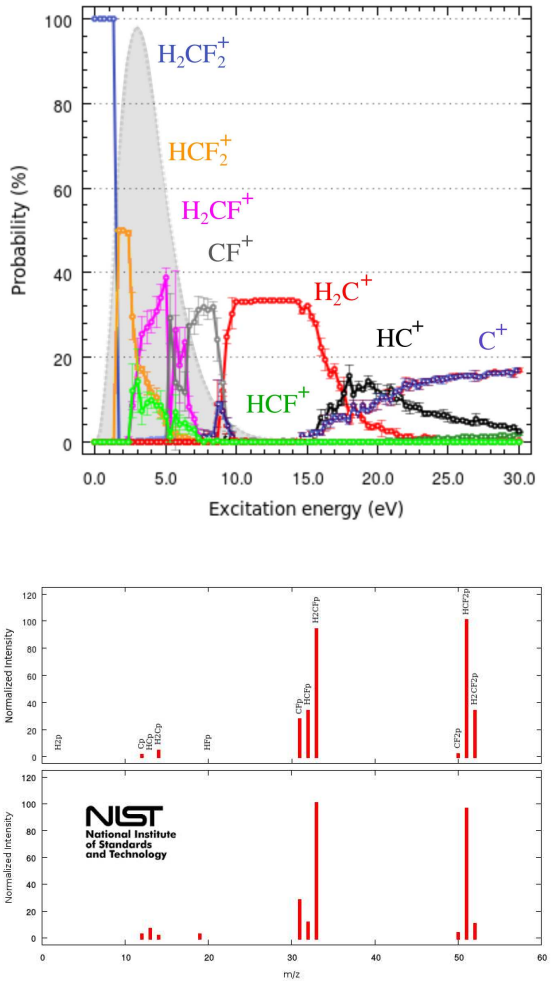

Figure 1. Fragmentation of CH_2F_2 molecule. Upper panel, breakup-curves. Middle/lower panel, theoretical/experimental [3] mass spectrum.

References

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