

Why are atomic and molecular dimers so exciting?

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Synopsis During the last 10-15 years, ion collisions have been used to unravel properties of van der Waals dimers from their fragmentation dynamics. This talk will review some recent highlights obtained in this field.

The large number of experimental and theoretical studies devoted to atomic and molecular van der Waals dimers for more than a decade is here to attest for their specific interest and the excitation they raised in the scientific community. One of their amazing feature is the monomers ability to interact at incredibly large distances through newly evidenced processes, due to the transition from closed to open shells upon ionization, such as Interatomic Coulombic Decay (ICD) [1]. However, this excitation is also due to the large amount of information obtained on the monomer themselves and in particular in the case of collisions with ions. Indeed, one of the first achievement has been to show that dimers behave as two quasi-independent monomers [2, 3].

Collision processes impact parameter dependent cross sections between an ion and an atom are not that easy to determine experimentally. The dimer geometry allows angular dependent measurements which give indirectly access to this impact parameter [3]. Dealing with molecules, the long standing question concerning the center to which the active electron belongs (could be reworded as “on which side of the molecule was the active electron during the interaction?”) has been answered thanks to the low electron mobility across an atomic dimer [3]. Furthermore molecular dimer fragmentation provides a smart way for metastable molecular state identification [4], one of the two monomers acting as a spectator probe to access the life time of the second monomer dissociating excited state.

Another strong motivation in studying ion-dimer collisions is to answer the question: to what extent gas phase results can be applied to the condensed phase. For example, can collision induced molecular fragmentation cross sections performed in the gas phase be used as the starting point (physical stage) for radiolysis chemi-

cal stage codes? Even if monomers tend to behave independently during a collision, interaction processes exist between them. Thus, while in low energy ion-atom collisions, electron emission vanishes, the ICD process appears as the projectile charge state decreases and becomes a new source of low-energy electrons. Such electrons are known to play a role in radiobiology and have to be taken into account at the end of the range, where the projectile ion stops in matter [5]. Van der Waals dimers mimic a simple environment while allowing keeping access to dynamics measurements using coincidence techniques such as COLTRIMS. However, it has also been shown experimentally that molecules may dissociate identically whether isolated or within a dimer [6]. This may validate the use of gas phase data in condense phase modelling.

Ion-dimer collision physics is rich and broad and has still plenty of topics to tackle. Theoretical calculations are just starting [7] and are highly needed to confirm the experimental data interpretations, as well as collision induced reactivity between the monomers within dimers [8].

References

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