Fragmentation of condensed diazenes

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Synopsis Electron stimulated desorption of anions and cations from diazine films is reported for impact energies of 0 – 80 eV, revealing resonances below and above the ionization limit and dipolar dissociation behavior.

To enable the information gathered in the gas phase interactions between electrons and molecules to be applied to the real life scenarios (eg radiotherapy), a clear understanding of gas and condensed phase interaction differences is necessary. Through condensed phase electron stimulated desorption1 (ESD) of analogues of DNA bases and radiosensitizers, we observe clear differences in the dissociative electron attachment (DEA) resonances and fragment appearance energies when comparing to gas phase experiments and calculations 2–4. These results can influence the modelling of electron transport in condensed phases and biological materials.

Our study focused on the molecules pyrimidine and pyridazine, both important to the field of radiotherapy5,6 and differing only by the location of the Nitrogen ring components.

The ESD involved condensation of vapors of each molecule on either a Pt or Ar substrate to form a submonolayer molecular target. Electrons of 0-80 eV are then incident on the film and the molecules fragment according to resonant or non-resonant processes. The desorbing anionic and cationic fragments are analysed via time of flight mass spectrometry.

We present differences in the desorbing fragment yields in the case of both anions and cations. Details in both type and appearance energy, and comparisons to previous observations are presented. Anion yield functions indicate that transient anions contribute significantly to molecular dissociation below 20 eV. This is via DEA and dipolar dissociation (DD), though the predicted low energy shape resonances do not appear to cause significant fragmentation in the condensed phase. The detected cations are the same species as seen in gas-phase mass spectra, albeit of differing relative intensity.

Figure 1. Desorption anion yields stimulated by 0 – 20 eV electron impact on sub monolayer quantities of pyrimidine condensed on an argon substrate at 18K

References

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