Final Report

Study of biological molecules by low- energy electrons.

Electron Induced Processing at the Molecular Level (EIPAM)
Exchange Grant
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PURPOSE OF VISIT

The purpose of my visit was bring experience with the high resolution electron beam that will be needed also for future experiments in Rome. In fact in our laboratory in Rome is in progress an apparatus consisting of an electron gun a collision chamber and quadrupole mass spectrometer with a nominal mass range of 532 amu. The hemispherical electron analyzer (HEM) will produce highly monoenergetic electrons with an energy resolution of approximately 0.05eV in the range between 0 - 15 eV.

DESCRIPTION OF THE WORK CARRIED OUT.

During my stay in the laboratory in Innsbruck in particular I was applied in the study of nitrotoluenes compounds by electron attachment .

Study of Nitrotoluenes by elettron attachment processes.

I investigated the interaction of low energy electrons with some nitro toluenes. Many proprieties of these substances and the fragmentation pathways of the molecular ion have therefore been extensively studied. In particular the 2,4-dinitrotoluene (DNT) and 2,4,6,-trinitrotoluene (TNT) have widespread applications as an explosive in both military and non-military fields. In fact their high electron affinity it allows the high probability of negative ion formation

A complete knowledge of the fragmentation paths produced by the dissociative electron attachment processes (DEA) may therefore allow the detection of explosive by the identification of negative fragment ions.

1.1 Experimental Setup

In these measurements a crossed beam apparatus for high electron resolution attachment is used [1]. The electron are produced by a filament and are accelerated with a lens system into a hemispherical electrostatic field analyzer, where the electron energy resolution is set a value 80 meV. After the hemispheres the electrons are accelerated and focused into a collision chamber where they interact with a neutral molecular beam. The formed anions are extracted into a quadrupole mass spectrometer and the ion current is amplified by a channeltron operated in pulse counting mode and recorded by a computer.

The energy scale and the resolution are calibrated by measuring the ion yield of a CCl_4 *gas calibration. In fact the ion yields of the anion for this gas exhibit a very sharp peak at 0 eV and a second peak at 0.8 eV.*

The vapour pressure of 2-mononitrotoluene (2MNT) and 2,4-dinitotoluene (DNT) were sufficiently high at room temperature but 2,4,6,-trinitrotoluene (TNT) had to be heated to about 60 ^{0}*C in order to obtain good signal. This is well below the temperature for thermal dissociation of the compound. The evaporated molecules effuse through a capillary into the collision chamber where they interact with a monochromatized electron beam.*

Description of the main results obtained

By accommodation of an extra electron into an unoccupied molecular orbital we have the formation of a transient negative ion M^- *.*

In the present experiments electron attachment to nitrotoluenes have been studied in the electron energy range from about zero to 15 eV. We could detect the following DEA reaction channels:

$$
\begin{aligned}
M + e^- \rightarrow\ M^{-(*)} \rightarrow\ & (M - OH)^- + \text{fragments} \\
\rightarrow\ & (M - NO)^- + \text{fragments} \\
\rightarrow\ & (M - NO_2)^- + \text{fragments} \\
\rightarrow\ & (M - OH - NO)^- + \text{fragments} \\
\rightarrow\ & (M - OH - NO_2)^- + \text{fragments} \\
\rightarrow\ & (NO_2)^- + \text{fragment}
\end{aligned}
$$

Electron capture leads to a variety of a further negative fragments. Fig1 and fig.2 show the ion yields of some fragment anions and are evidents the differents positions of resonances observed . The fig.4. shows the incident electron energy dependence of the produced fragment anions $(NO_2)^-$ from the three different gas phase esplosive molecules. The figure indicate clearly differents resonances in the low electron energy range.

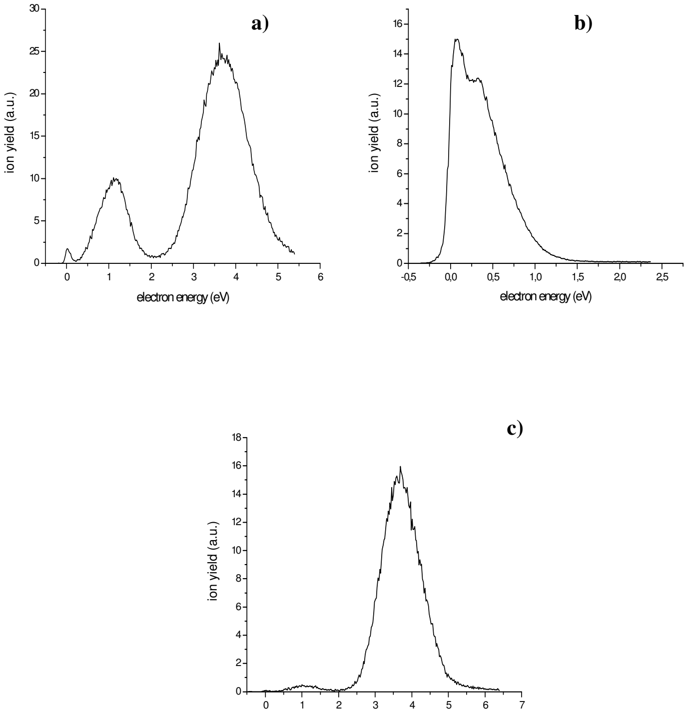

Figura 2 _ *Ion yield for (M-NO)$^-$ formation in* **a)** *2-monotoluene (2MNT).* ***b)****2,4-dinitrotoluene (DNT).* ***c)****2,4,6- trinitrotoluene (DNT).*

For the 2MNT has been possible to estimate the absolute cross by taking the know cross section of second peak (0.8 eV) to electron attachment CCl_4 as calibration standard and comparing with the 2MNT$^-$ count rate. Assuming similar detection efficiencies for CCl_4 and 2MNT$^-$ and by estimatine the partial pressures, the cross section is evaluated to be $\approx 10^{21}$ cm^2 (accuracy within 1 or 2 order of magnitudine) at the peak of the dominant sharp resonance around 0 eV (fig.5) . The cross sections for the other nitrotoluenes have not been possibile evalueted because of the lower vapour tensions of DNT and TNT.

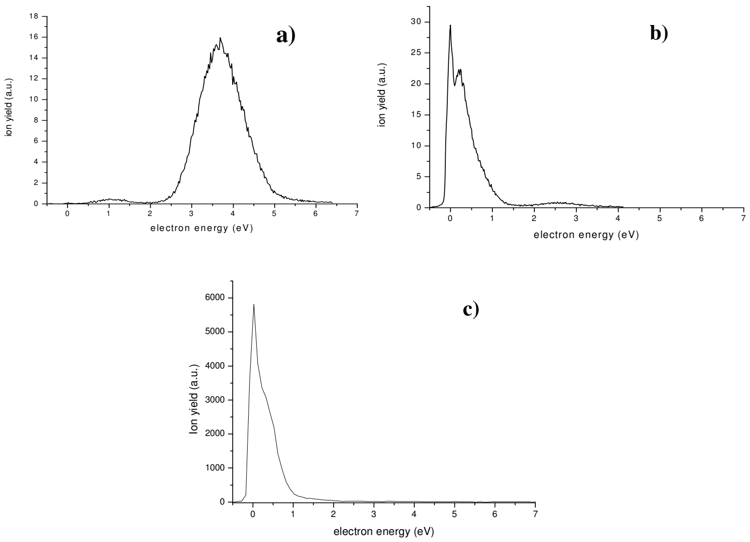

Figura 3_ *Ion yield for (M-OH)⁻ formation in* **a)** *2-monotoluene (2MNT).* ***b)****2,4-dinitrotoluene (DNT).* ***c)****2,4,6-trinitrotoluene (DNT).*

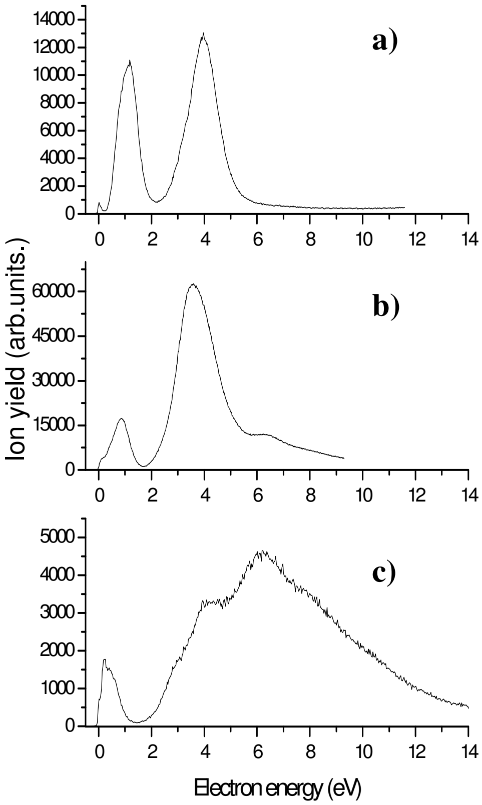

Figura 4_ *Ion yield for NO_2^- formation in* **a)** *2-monotoluene (2MNT).* ***b)****2,4-dinitrotoluene (DNT).* ***c)****2,4,6- trinitrotoluene (DNT).*

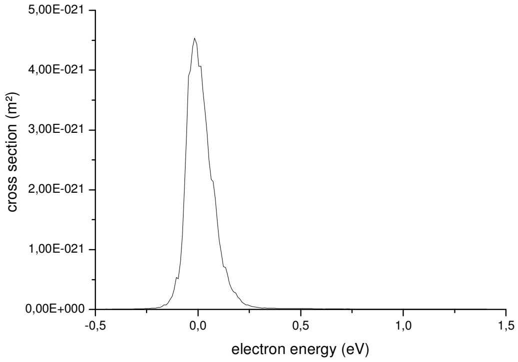

Figura 5_*Absolute cross section of 2MNT ⁻*

The present gas-phase experiments confirm strong decomposition of nitrotoluenes into fragments anions and neutral radicals at low electron energies (0-15 eV).

An important application of resonant dissociative electron attachment had pointed out in these previous results. In fact we could confirm the possibility to estimate the presence of different kind of explosive molecules by the detection of the resonances of the fragment NO_2^-.

This project is supported by Detection Technology Department Fort Halstead Sevenoaks .

Future Collaboration

I would you like to thank to EIPAM programe to partecipate in this work , in particular all group of Prof.T.Maerk and Paul Scheier. I hope in the future to have the possibilty to come back in Innsbruck. In fact the present project is a collaboration between the Laboratory of Kinetics and Laser Photochemistry at the University of Rome La Sapienza and the Institut für Ionenphysik at the University of Innsbruck.

[1] Muigg,D; Denift,G; Stamatovic, A; Mark, T.D. Chem. Phys. ***1998****, 239, 409.*