Gas phase molecular physics experiments in synchrotron sources of second and third generation

Wednesday 24 Nov 2010 at 13:10 (00h30')

This talk will present an overview of gasphase experiments of molecular and atomic photoionization from the the standpoint of a user. The studies presented are specifically devoted to the study of single and double photoionization processes as well as photoelectron angular distributions. In addition to a brief overview of the physical processes studied, this presentation will have a stronger focus on the requierements and needs, both in terms of flux and resolution, that these studies pose to experimental beamline where they are carried out. A comparison of performance of experiments carried out at a second generation source and a third generation source will be presented, taking the autovibrational processes in H2 as a concrete example.

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Co-authors :

Presenter : Mr. JUAREZ-REYES, Antonio (Instituto de Ciencias Físicas UNAM)

II Mexican Workshop on Accelerator Physics: A Light Source

Puerto Vallarta, 2010

Gas phase molecular physics experiments in synchrotron sources of second and third generation

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Scope

1.- Energy resolution and flux needed for high resolution molecular spectroscopy.

1.1Molecular Photoionization and spectroscorpy
1.2 What do one needs to do high resolution molecular spectroscopy?
1.2 Features of some sources where this capability is available.

2.- Case studies to illustrate the point: Single and double Photoionization and photoelectron spectrocopy.

3.- Other brief examples and future prospects .

1.3 What does the future holds, and what do one need in this field to try and reach for it.

Molecular studies, what for?

1.-The study of molecular dynamics has the aim of finding out

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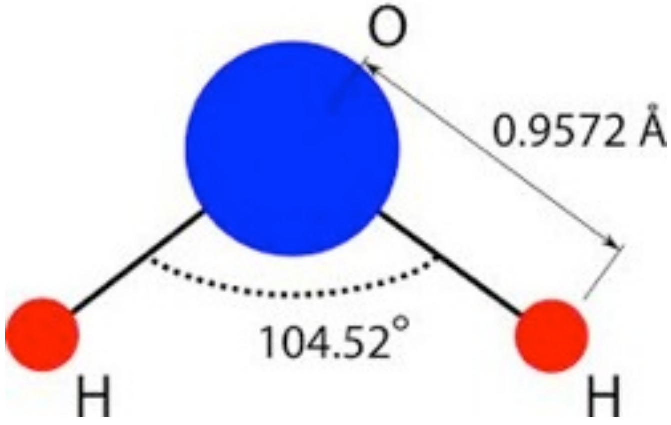
-Bond lengths,



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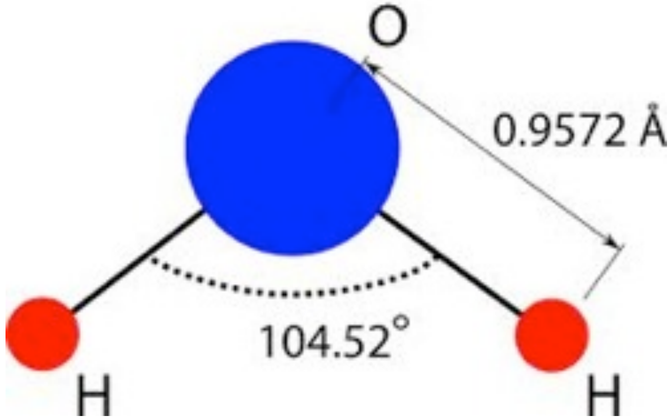
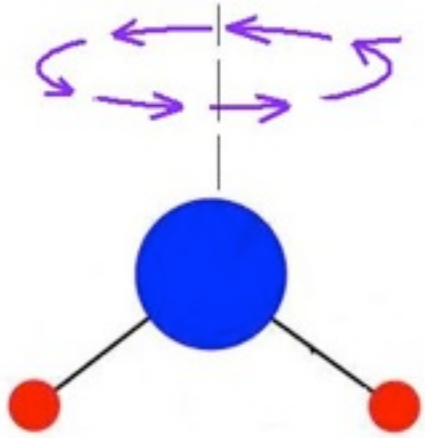
-Molecular inertia moments,





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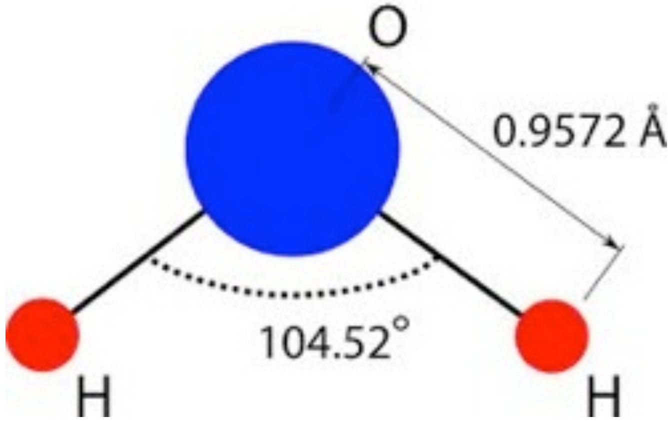
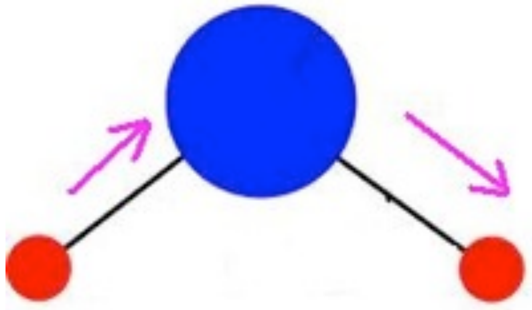
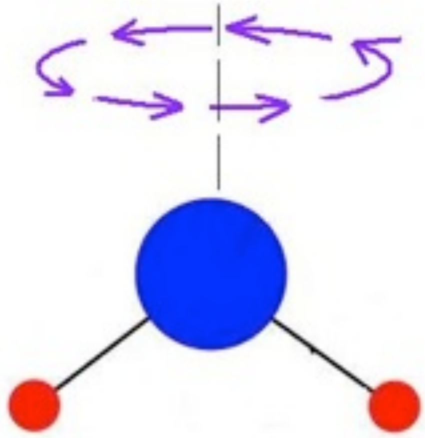


-Bond lengths,

-Molecular inertia moments,

-Force constants of bonds,





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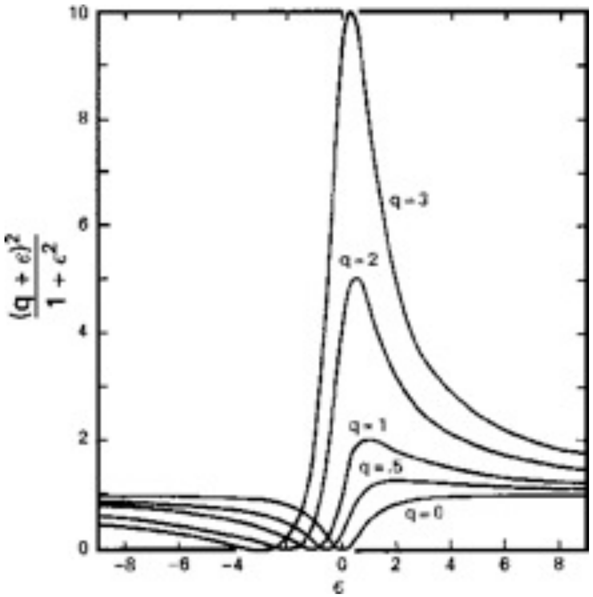

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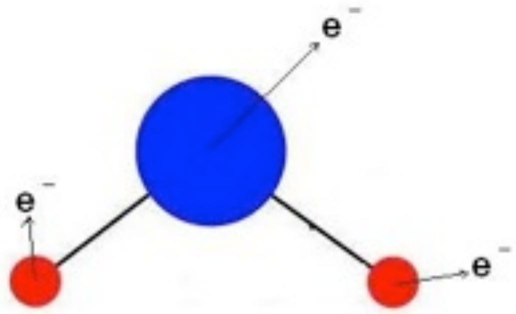

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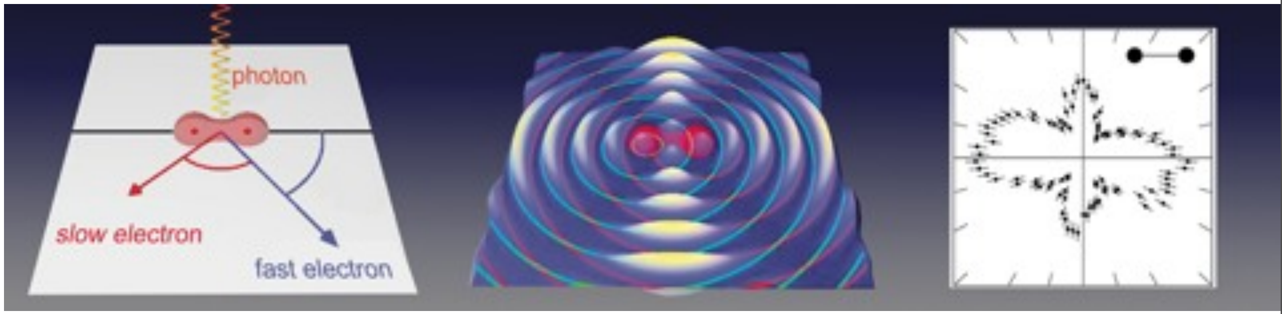

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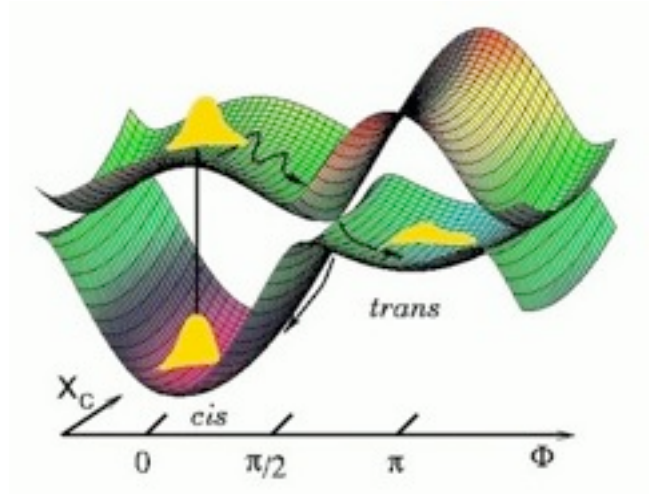
- Temporal dynamical evolution of electrons and nucleii in molecules



1.-Energy resolution and flux needed for high resolution molecular spectroscopy.

Molecular spectroscopy is an active field in synchrotron radiation sources (where low photon energy range is available). i.e. from 10 eV and higher.

Daresbury SRS, England, 2nd Generation

Sincrotrone Elettra, Italy. Third Generation. + Fermi

Advanced light source, Berkeley, USA. Third generation

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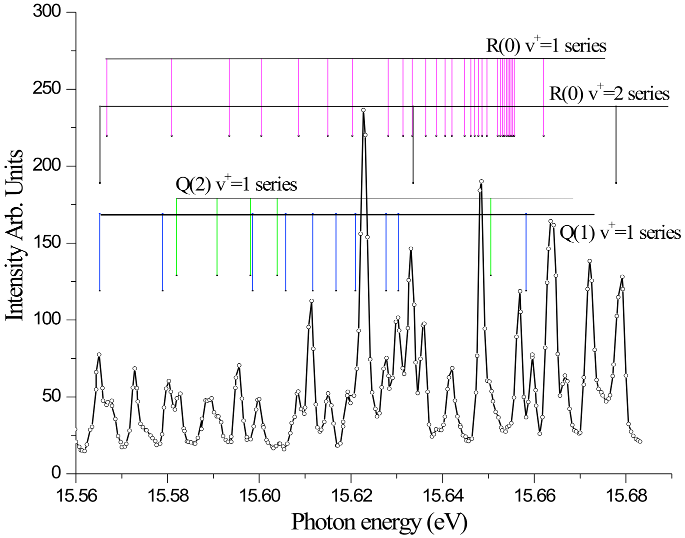

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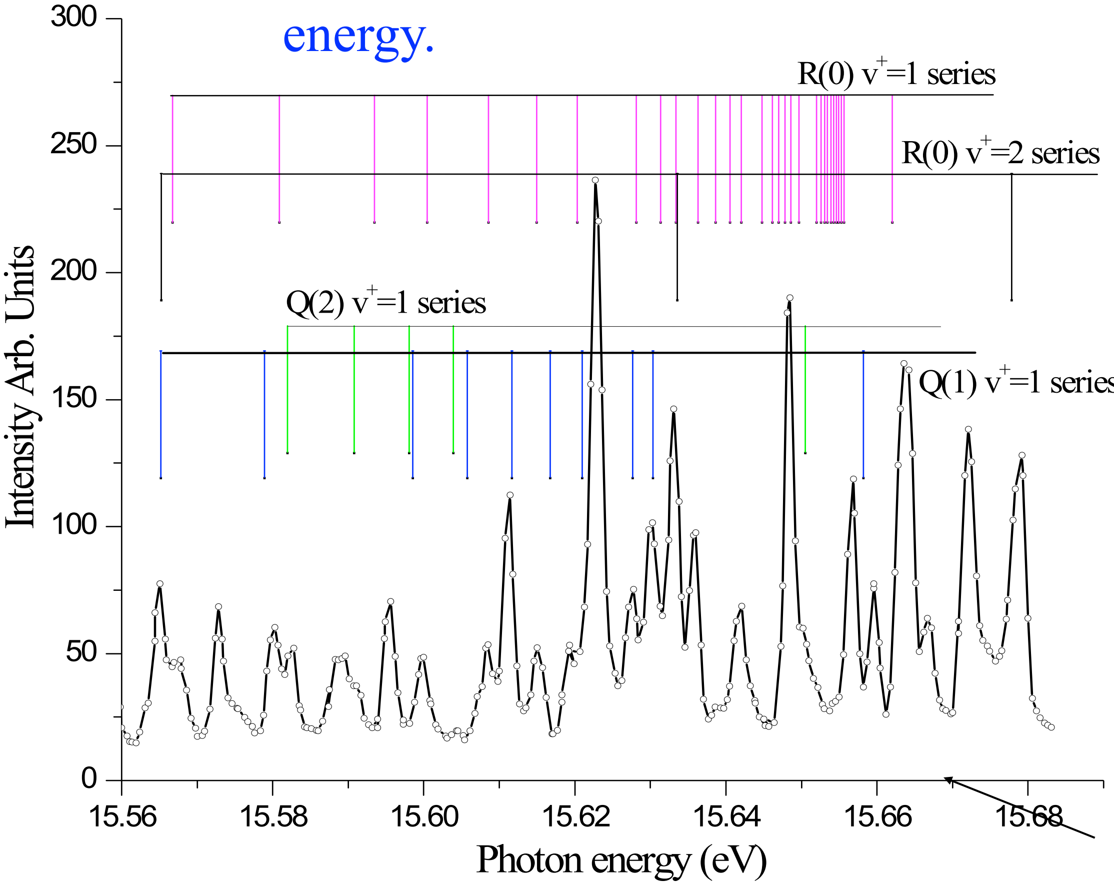
Molecular spectroscopy usually involves studying the yield of electrons, ions and fluorescence as a function of incoming photon energy.



Ion yield as a function of photon energy, ortho D2

The photoionization cross section of several molecules usually presents a wealth of structure, that one would like to resolve

assign and understand.

The snag being that total cross sections are usually rather small.

.048 Mb -28

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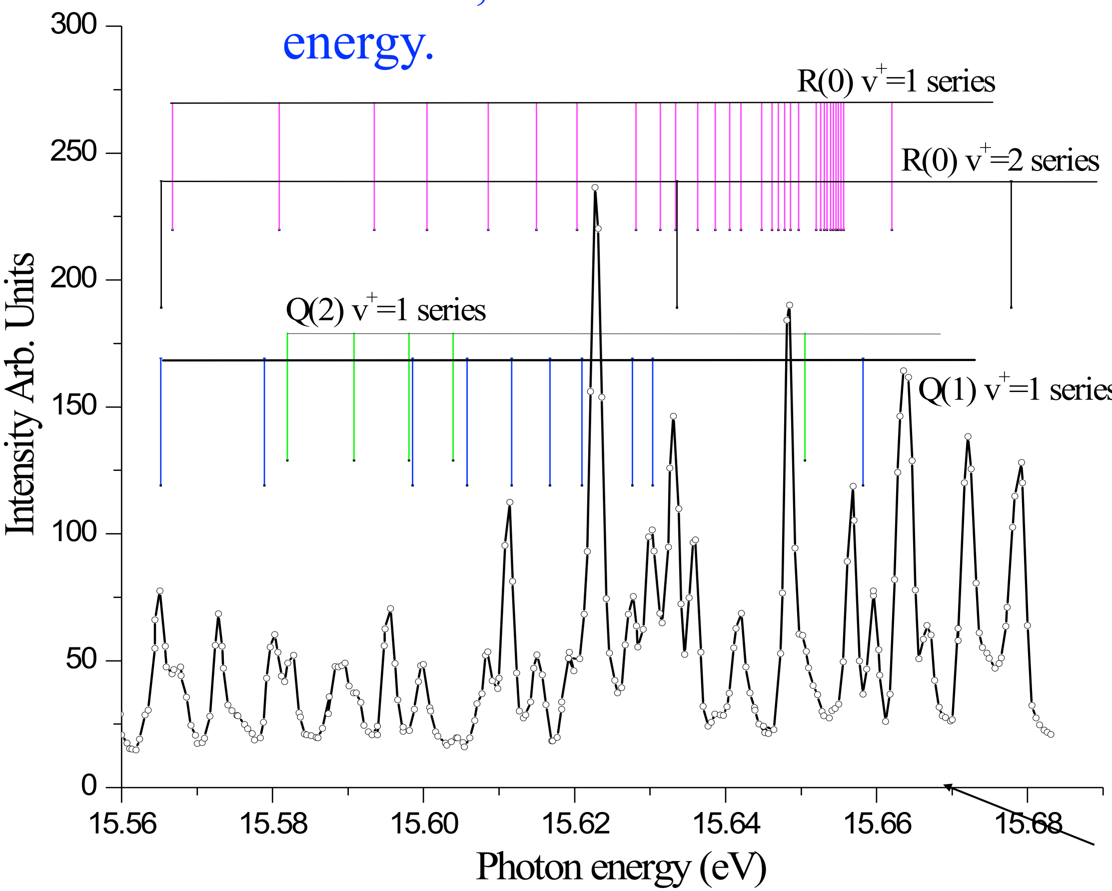

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D_2 Cross section

Electron Impact= 8.5 x10^{-18} cm ^{2}

Photoionization: .048 x10^{-18} cm ^{2}

.048 Mb -28

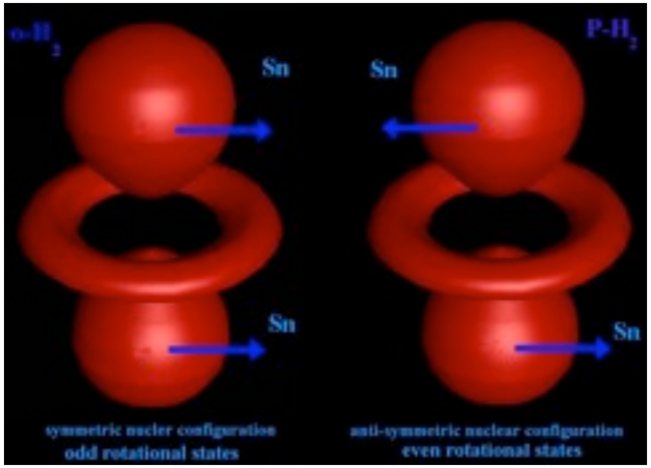
1.-Energy resolution and flux needed for high resolution molecular spectroscopy.

These two – often competing – requirements: **high photon energy resolution and high flux**, are one of the main compromises one encounters when doing molecular spectroscopy at synchrotron radiation sources.

Other desirable features that a synchrotron Source should have, for AMO physics are:

-Dependability (A stable source over several Hours)
-Good polarization characteristics (good in third generation sources, not so good in second generation SRS)
-Possibility of single bunching (for time dependent experiments)
- Good technical support (a synchrotron is more than relativistic electrons, the end station and the people behind it are central!)

2.- Case studies to illustrate the point: Single and double Photoionization and photoelectron spectrocopy.



Examples

Double and single Photoionization of H_2O SO_2, NO2. The double with the toroidal, the single with the Mc Pherson (Daresbury SRS)

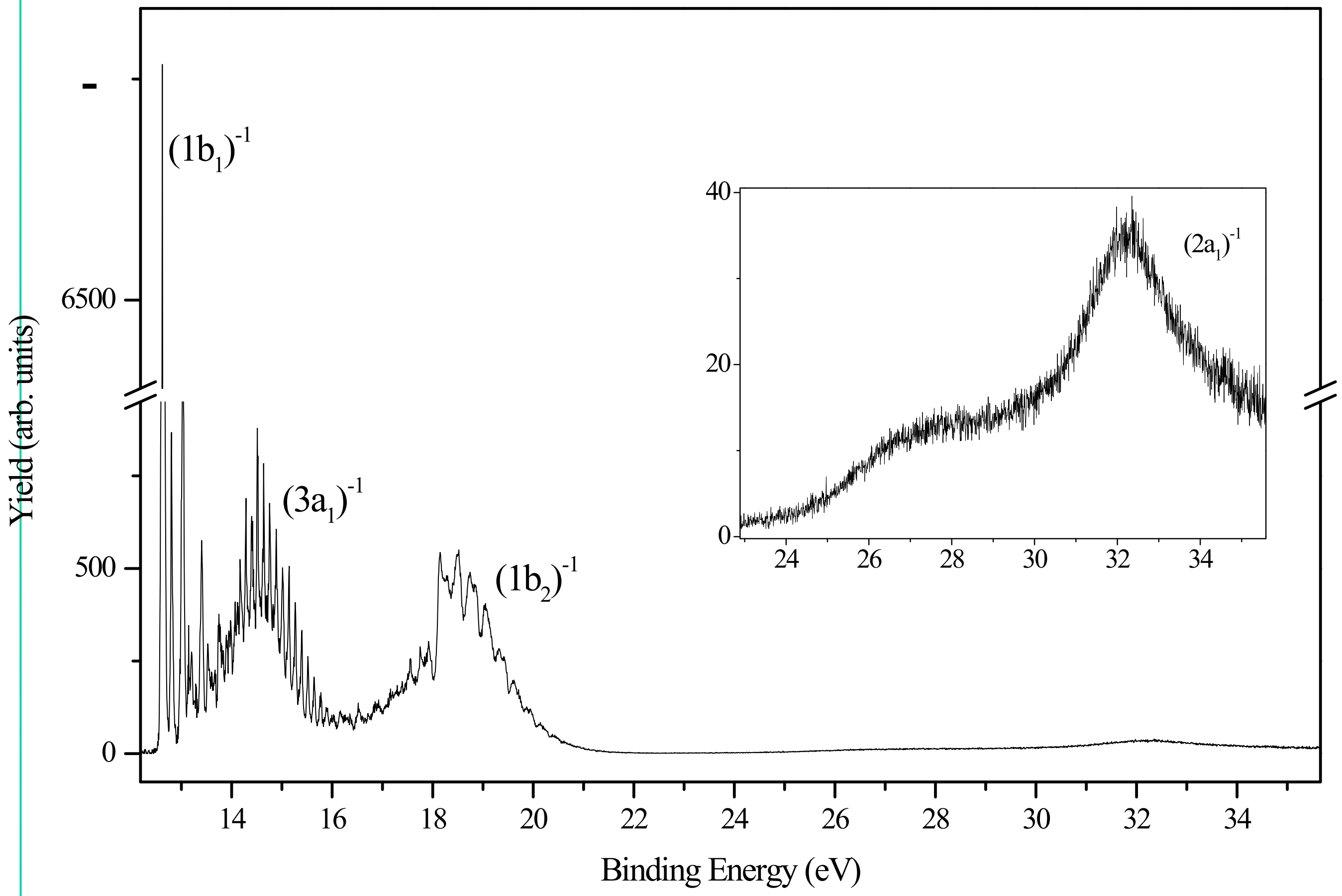
H2 spectra at Daresbury and Trieste, Elettra, sumary of transitions with high angular momenta (Elettra, Trieste)

He Satellites and VMI

Double and single Photoionization of H_2O SO_2, NO_2.

Daresbury SRS second generation source
Cheshire, England, closed 2004

1.- Single Photoionization studies of water with a Mc Pherson monocrhomator, using the Threshold Photoelectron Technique



cross section .3 to .7 x10^{-18} cm ^{2}**. Spectra taken in 8 hrs**

1.- Estudios de ionización doble y simple con luz sincrotrón

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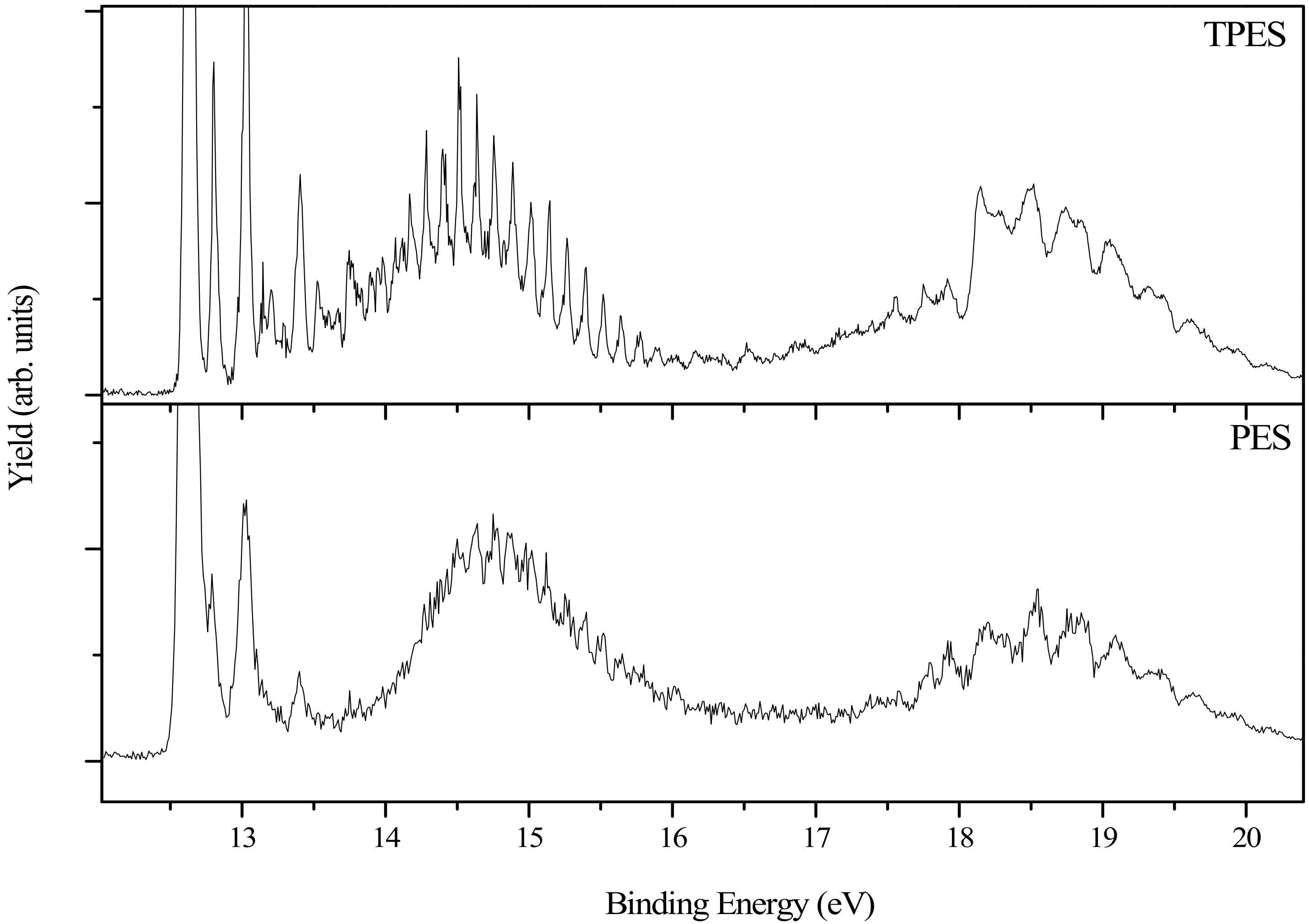
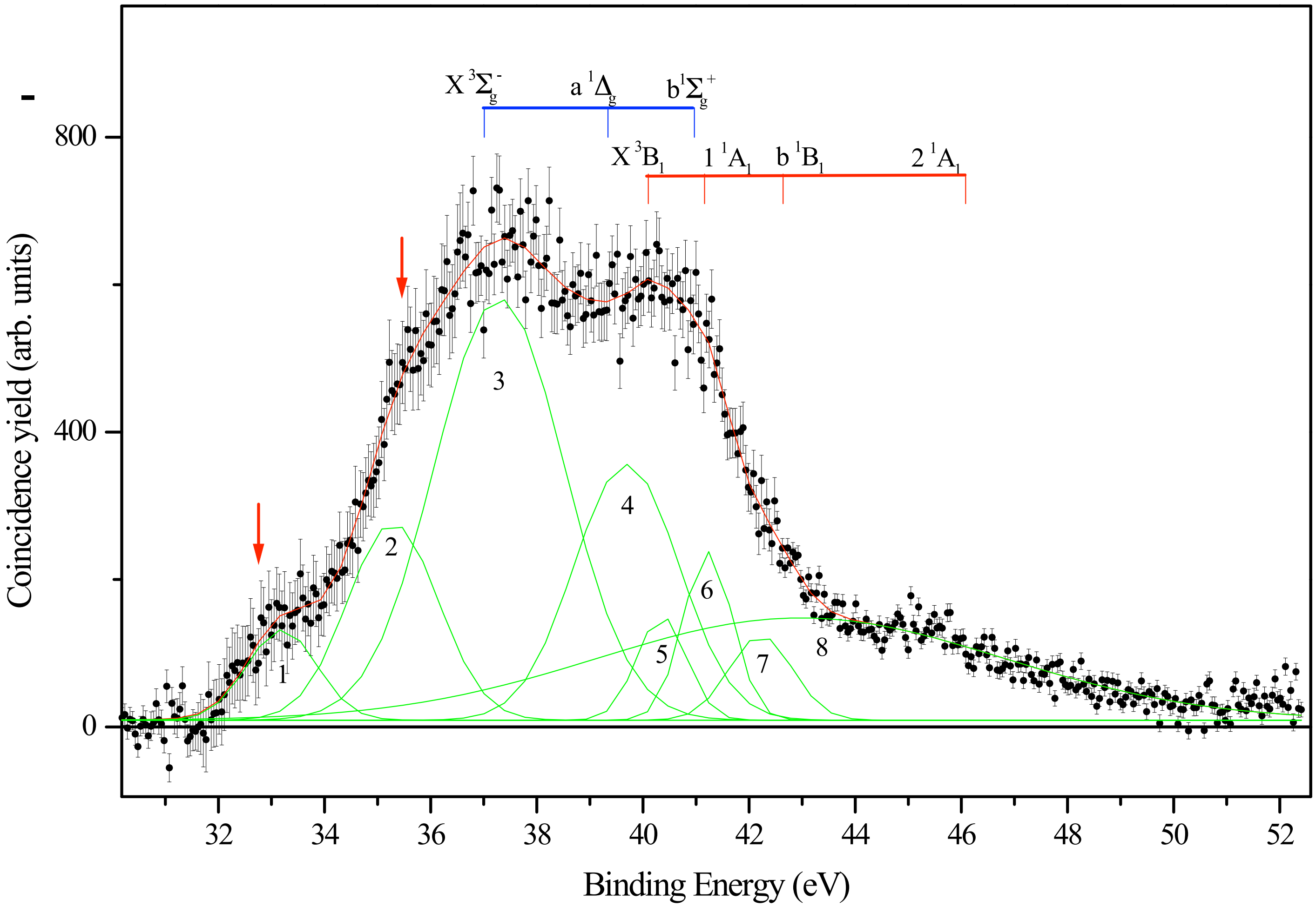


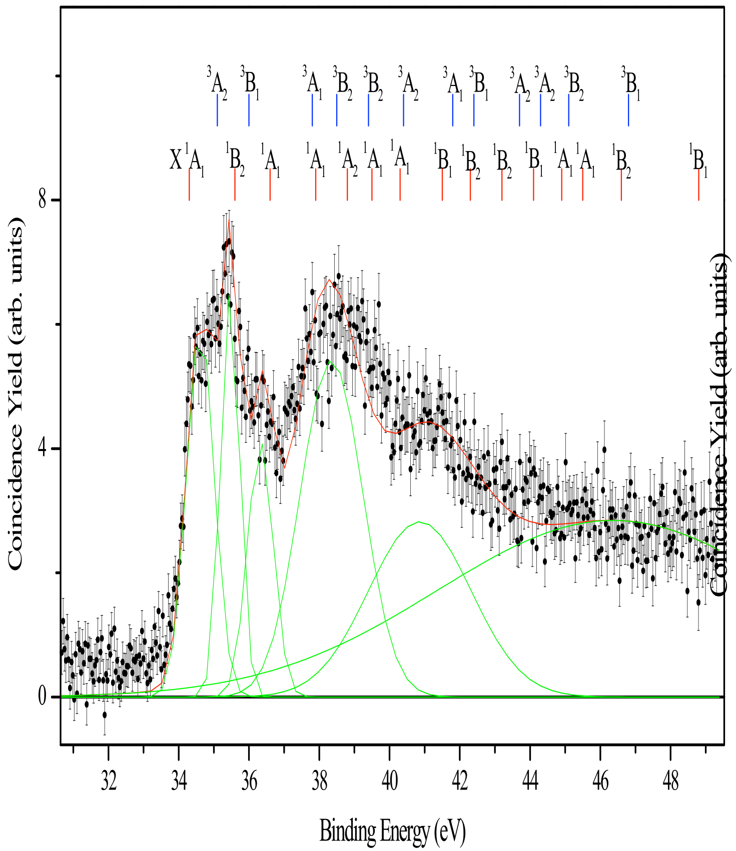
1.- Double photoionization using a Toroidal Grating Monochromator (H2O)



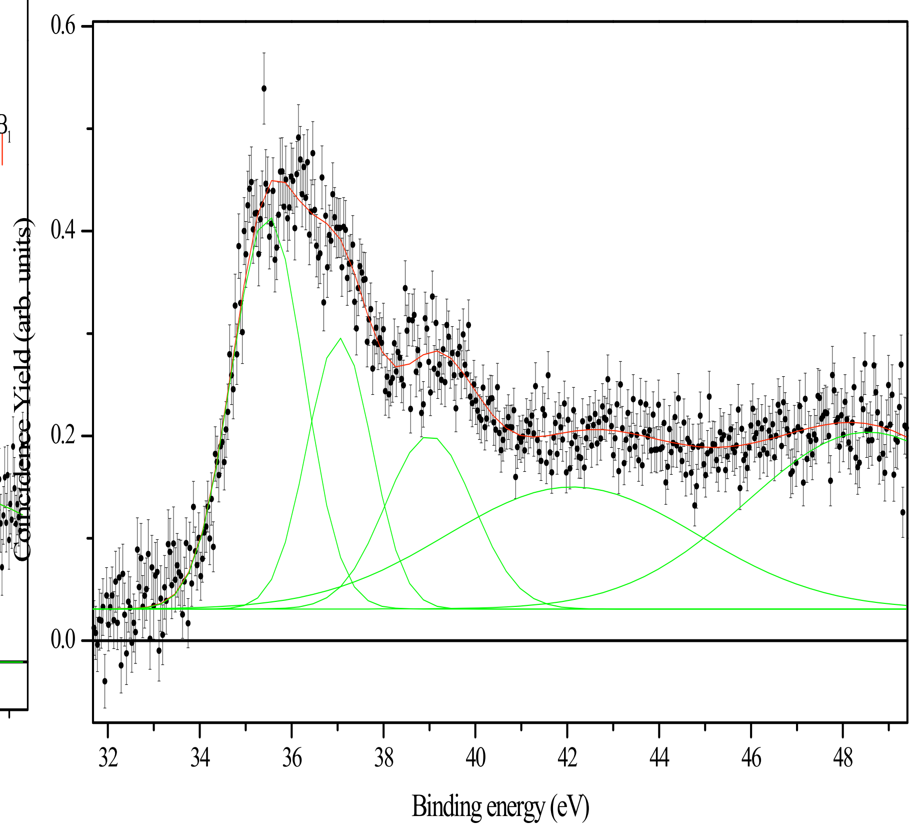
cross section .015 $\times 10^{-18}$ cm^2**. Spectra taken in 4 days**

Algunos resultados

Double photoionization of SO2



Double photoionization of N2O



Other measurements

Double photoionization of HBr and HI at Daresbury.

The spectrum shows the structure of the metastable states of the doubly charged ion

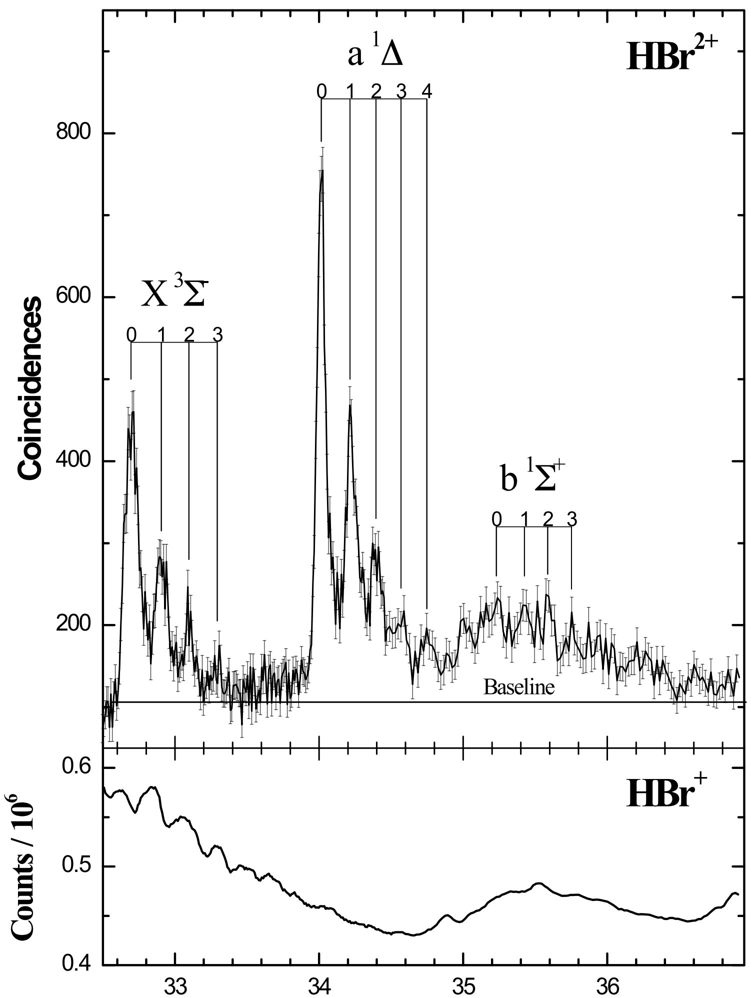
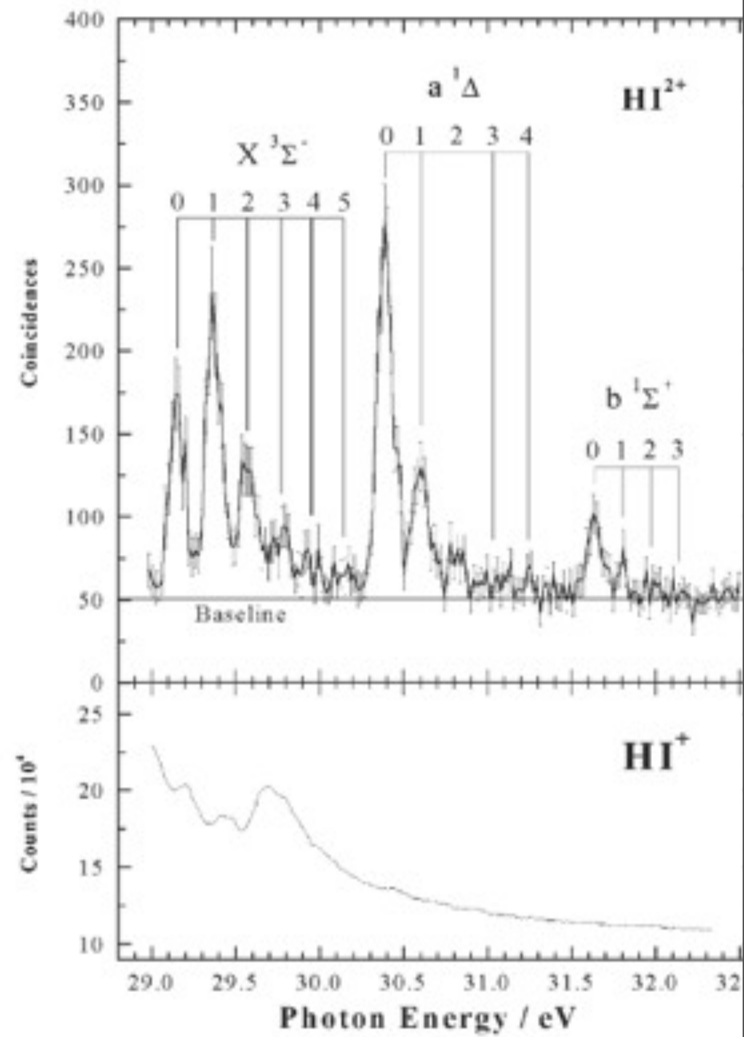
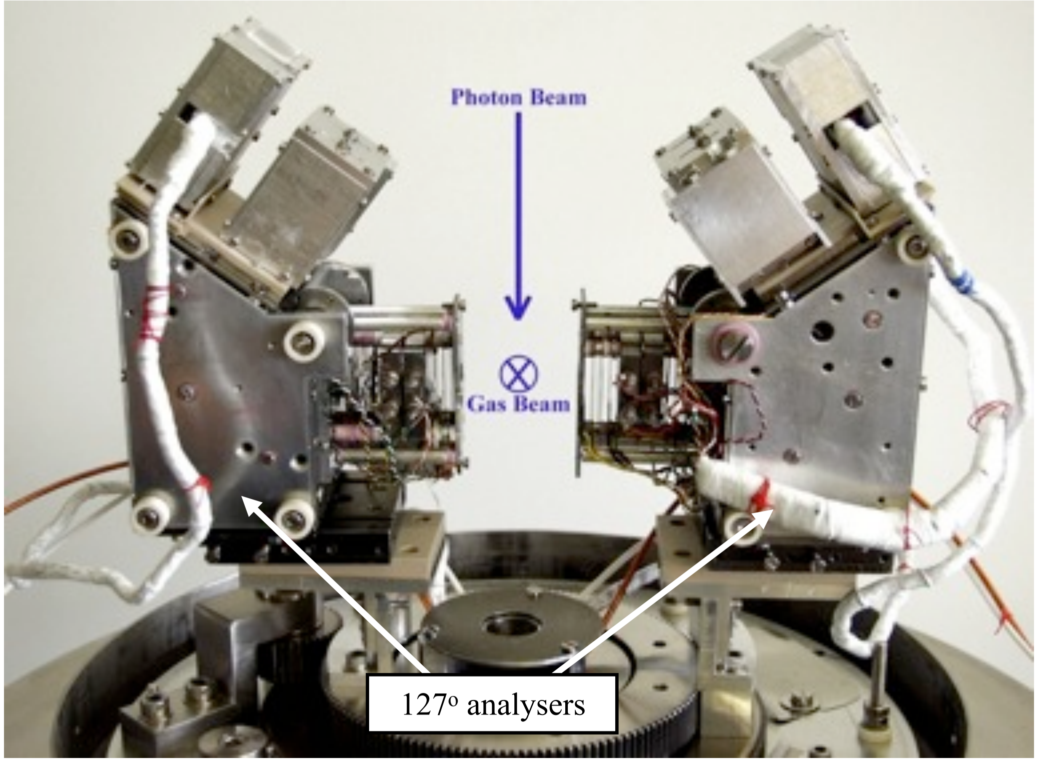


Fig. 1



1.- Estudios de ionización doble y simple con luz sincrotrón

-These measurements were aided by the use of high collection energy spectrometers



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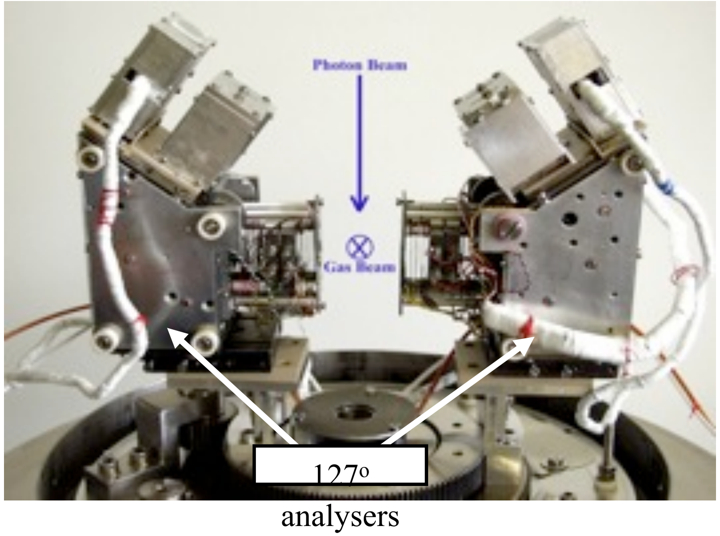

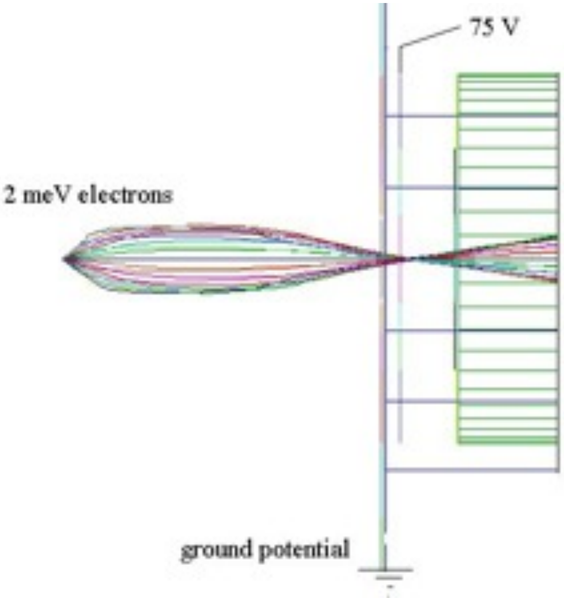

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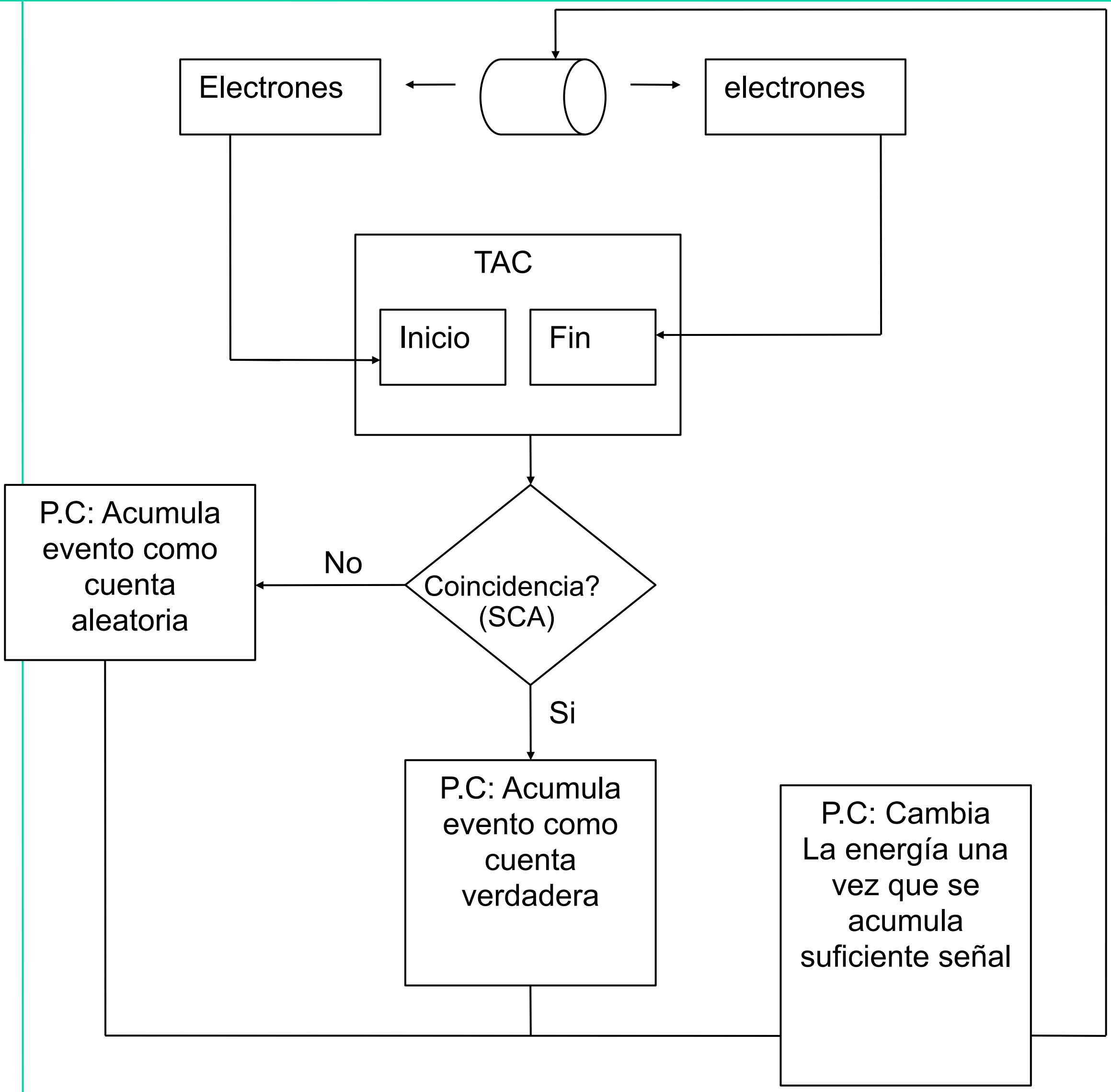
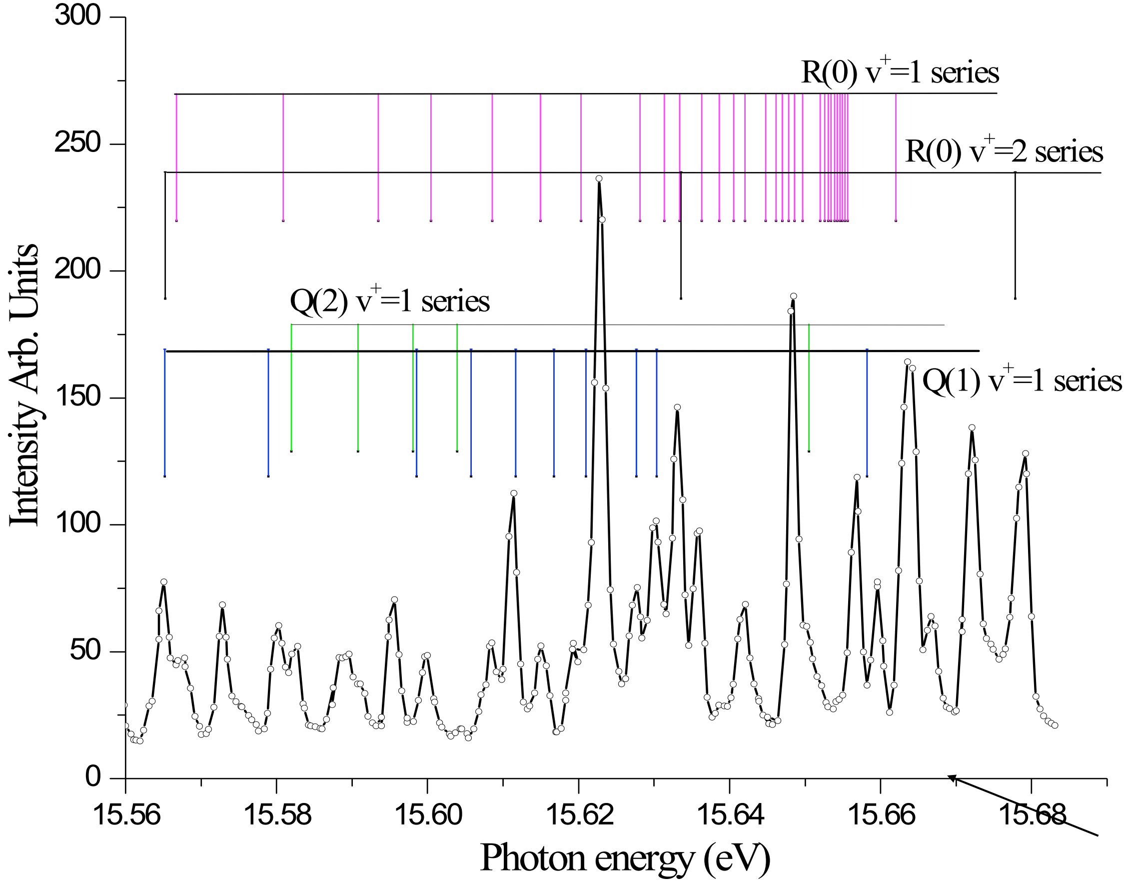


La clave Para distinguir los fenómenos de ionización doble es emplear un circuito de coincidencias

Elettra, Trieste, third generation source

1.-Energy resolution and flux needed for high resolution molecular spectroscopy.



D_2 Cross section

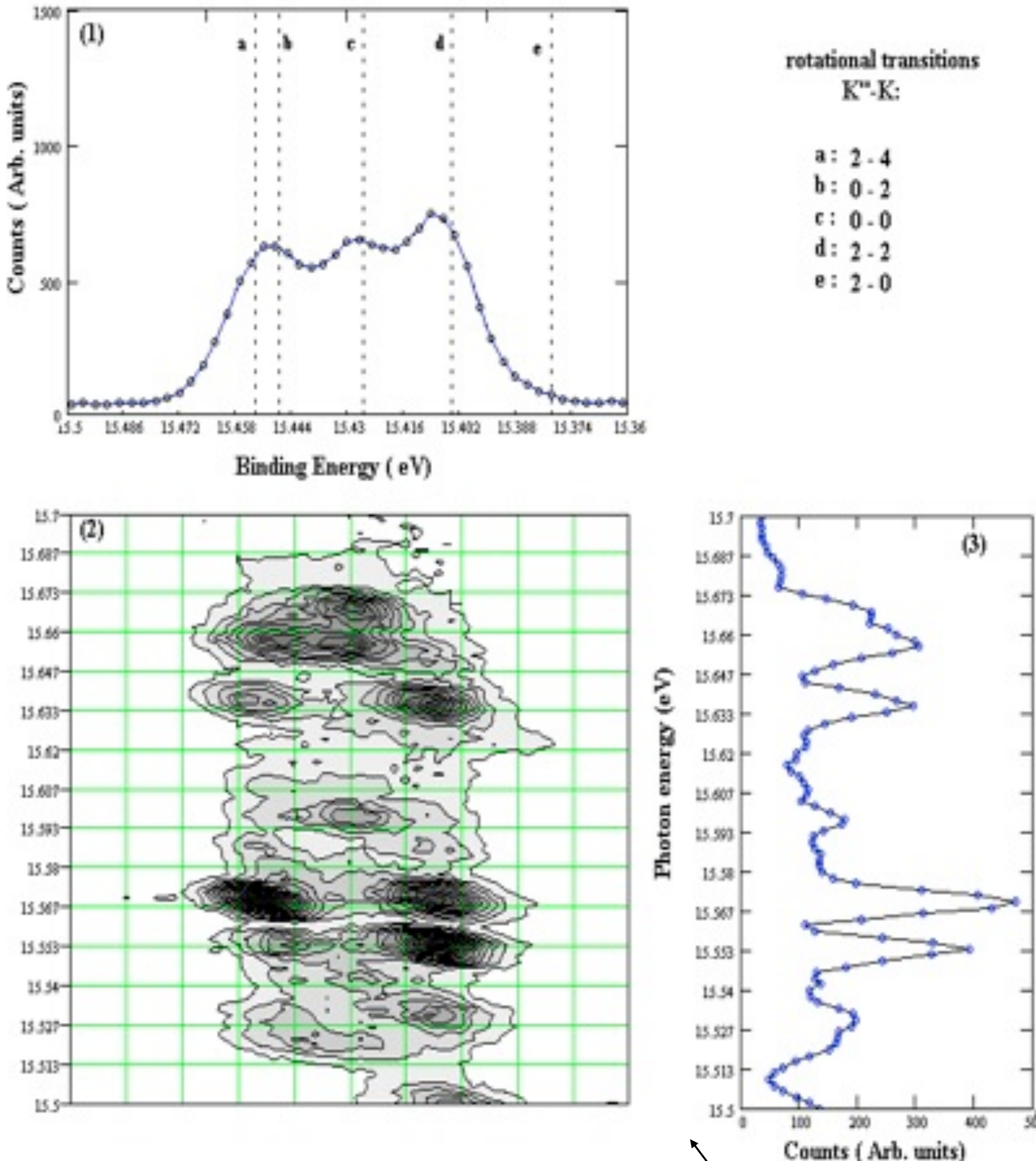
Electron Impact= 85 x10^{-18} cm ^{2}

Photoionization: .048 x10^{-18} cm ^{2}

Ion yield as a function of photon energy, ortho D2

.048 Mb -28

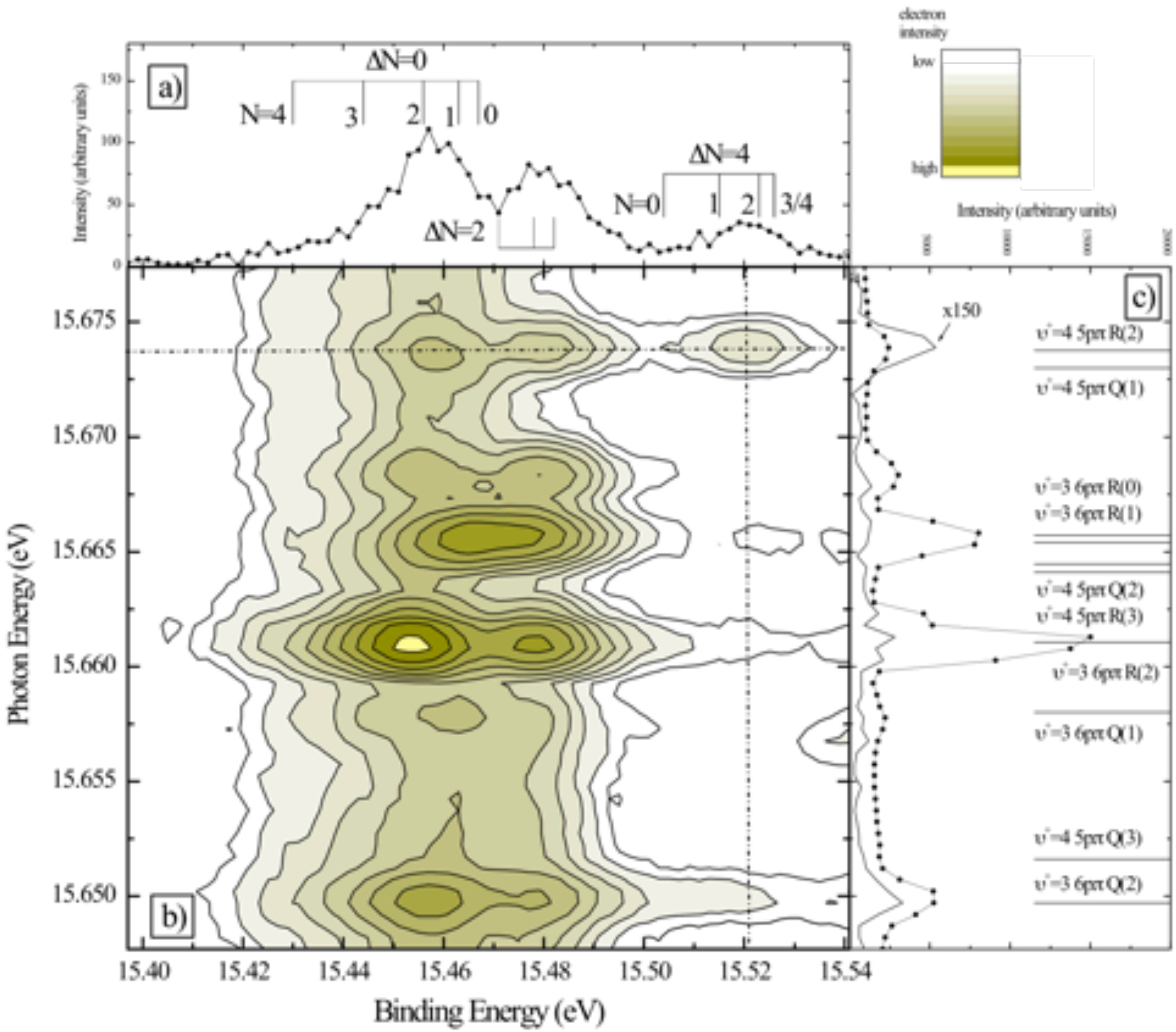
Vibrational autoionisation in D_2



Decay paths as surveyed with the McPherson at Daresbury (3 days)

ΔN **ΔN**

Similar measurements taken in 2 hrs at Elettra.



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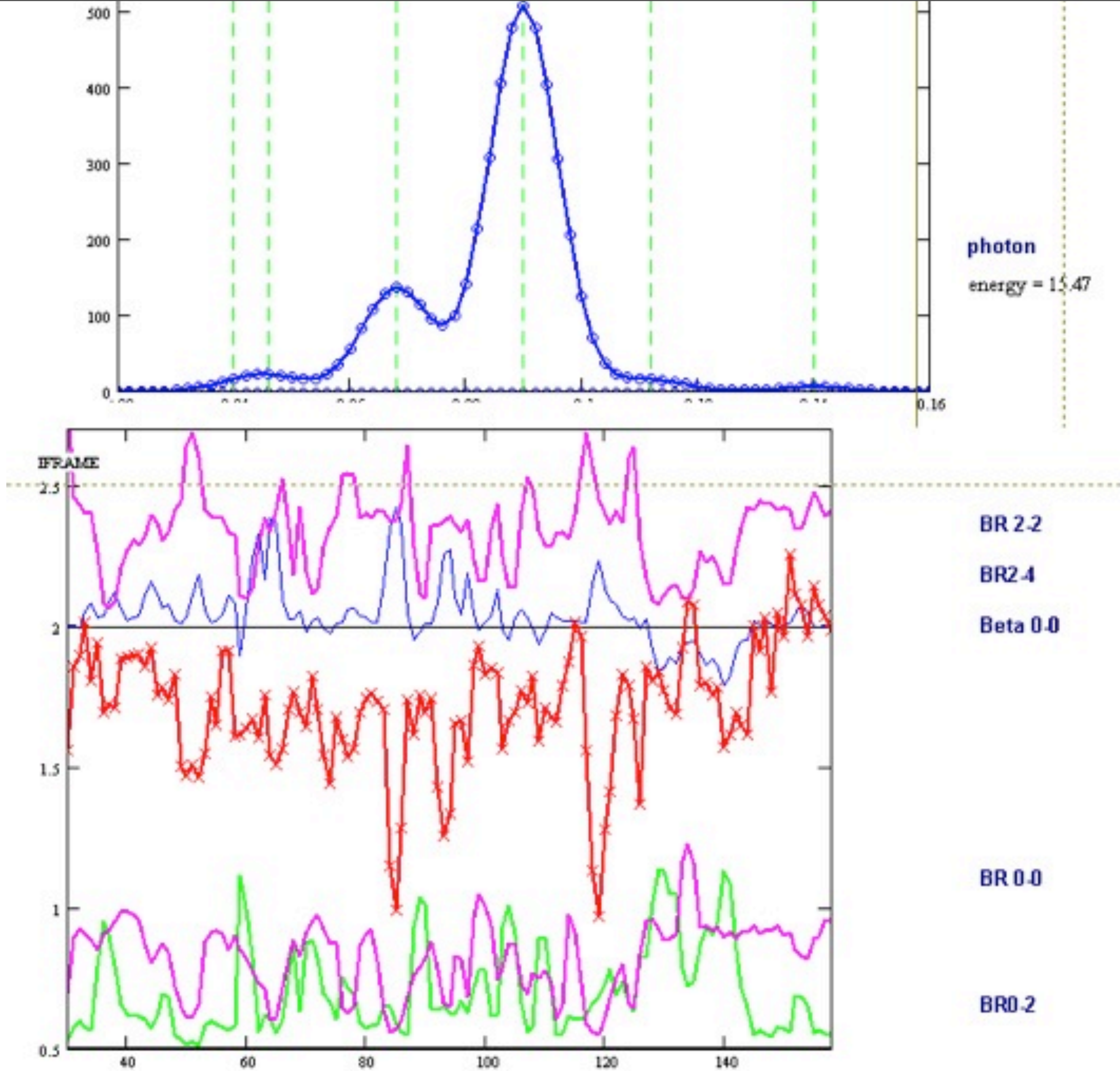
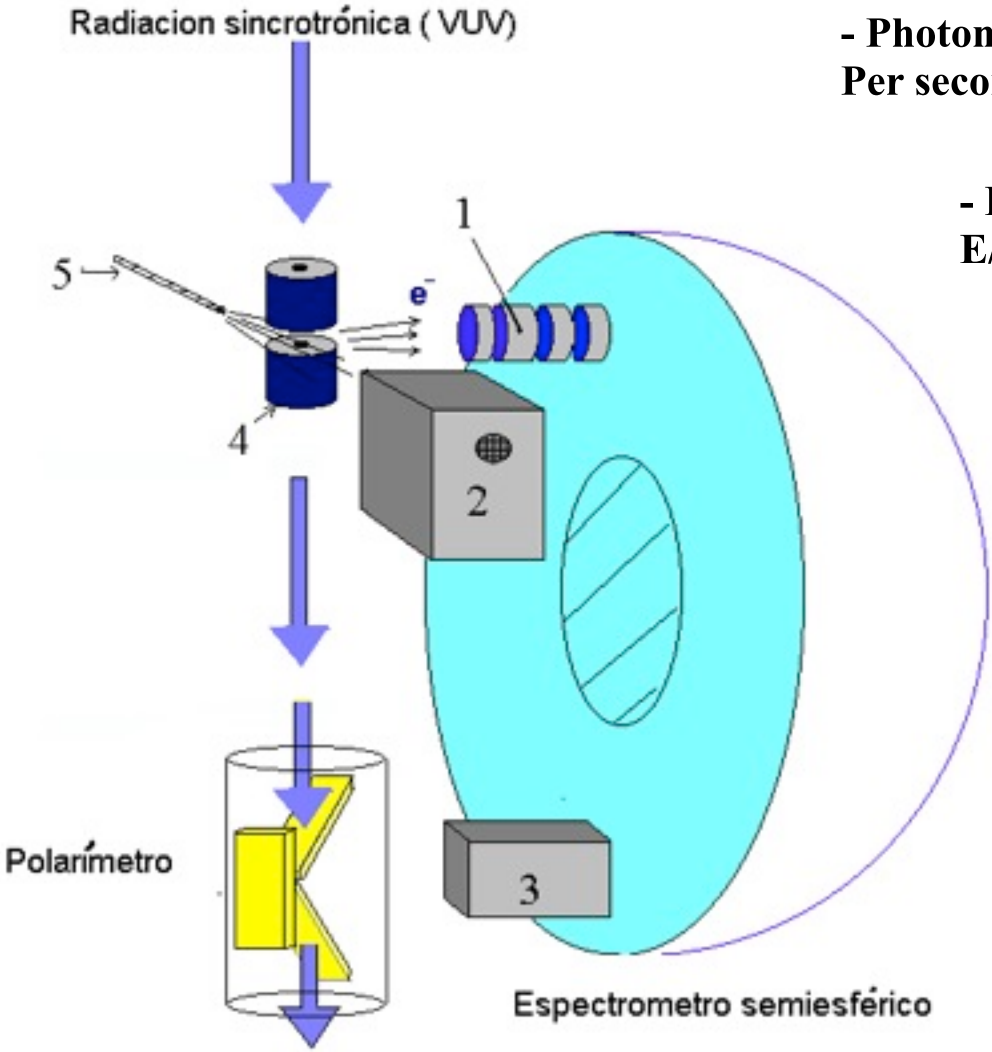


photon
energy = 15.47
IFRAME
BR 2-2
BR2-4
Beta 0-0
BR 0-0
BR0-2

A case study to illustrate the point: Photoionization and photoelectron spectrocopy in ortho-D2. 2.2 2.2 What do you need to see the process



- Photon flux: In the order of 10^{14} photons Per second/cm^2 - **Flux must be stable over hours.**

- Resolving power E/ΔE=15000 **Over a variable photon range**

- Photoelectron energy resolution of 6 to 7 meV (a stable, photoelectron spectrometer) **It needs some days to set up and condition**

- Catalytic sample Preparation in situ Of ortho D_2. **Fairly good technical support in cryogenics and vacuum to do your thing**

3.- Other brief examples and future prospects

Photoionization of ablated clusters

In addition to fundamental studies of molecules, molecular techniques at synchrotron sources, one can study the photoionization of clusters

Photoionization of ablated clusters

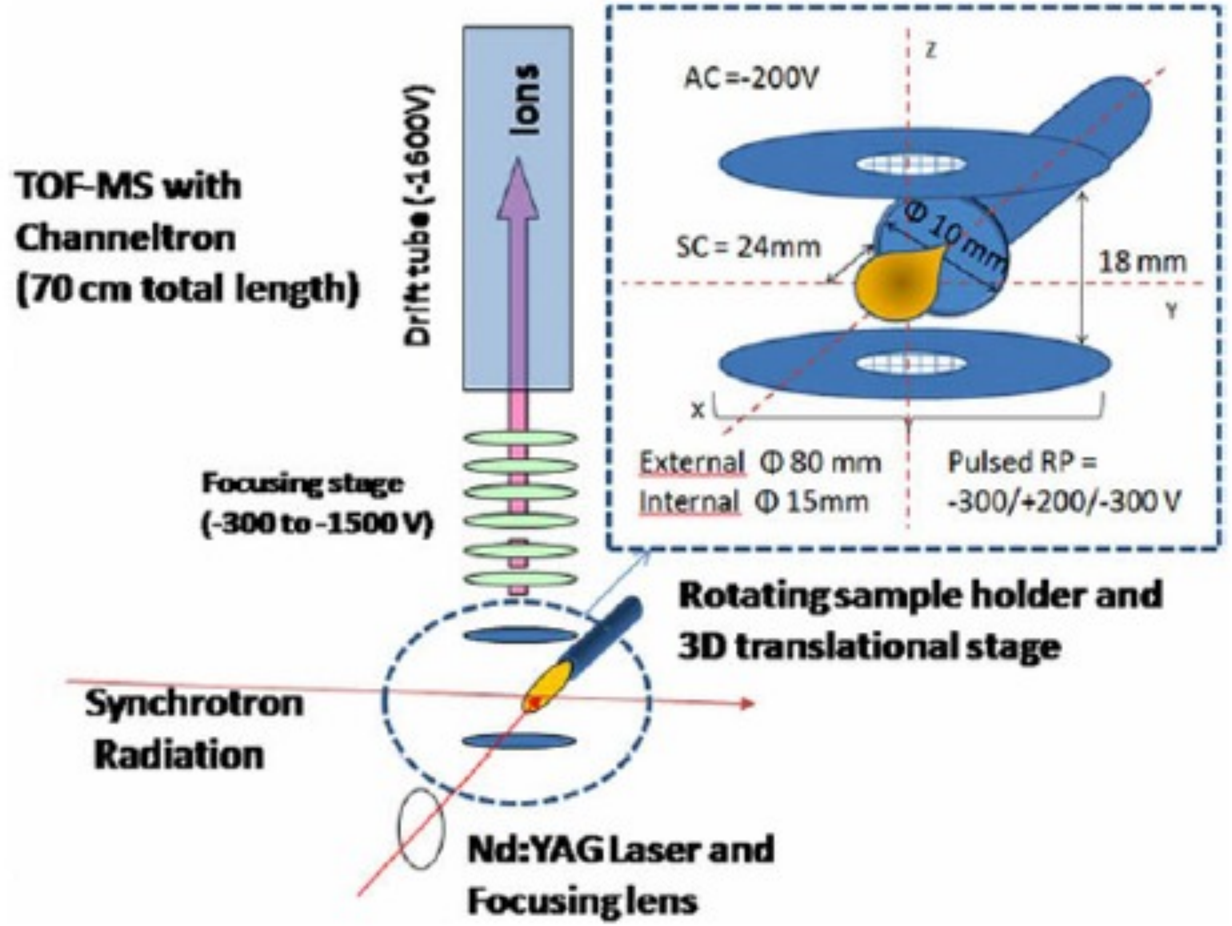


Fig. 1. Scheme of the apparatus to laser ablate a solid sample and to detect ionized species by the synchrotron light. The inset shows a detailed picture of the interaction region and lengths (AC – accelerating plate; RP – repelling plate; SC – source to centre distance).

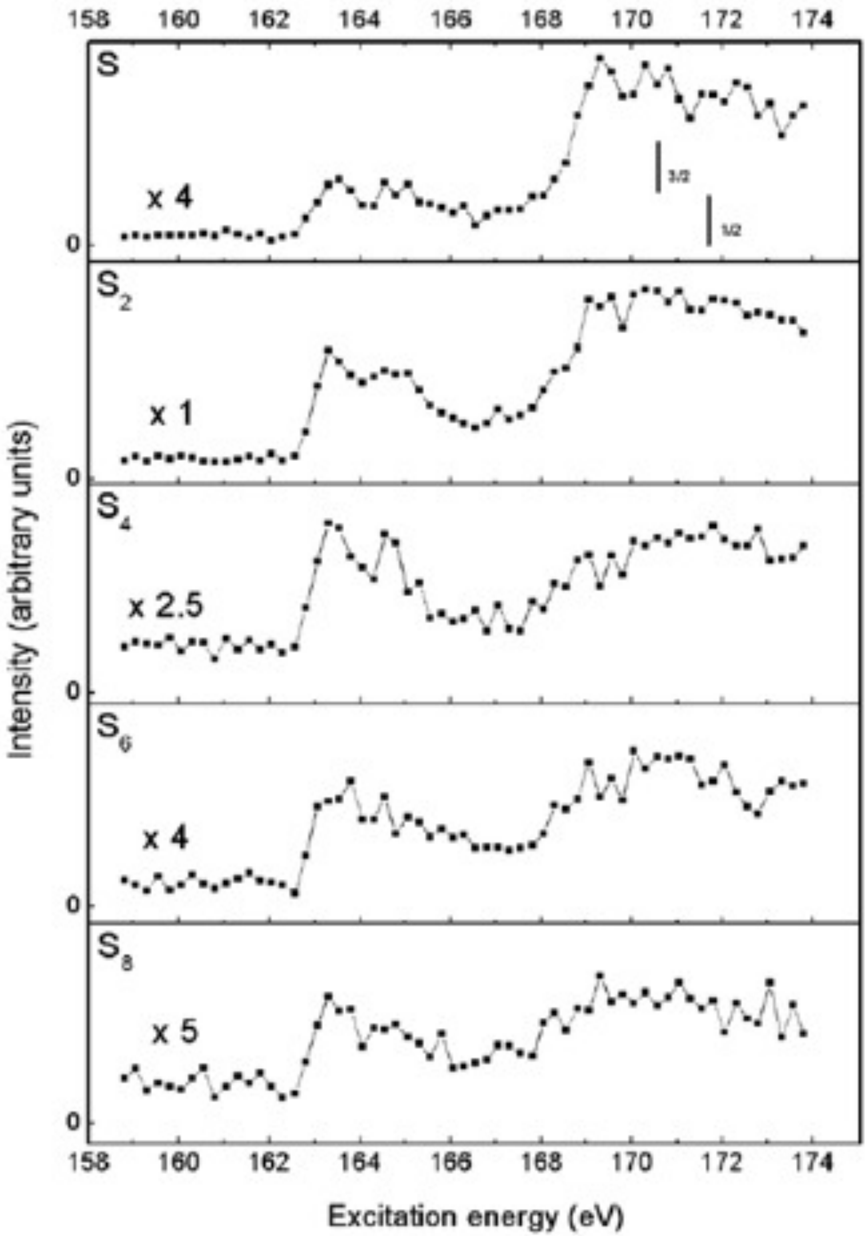
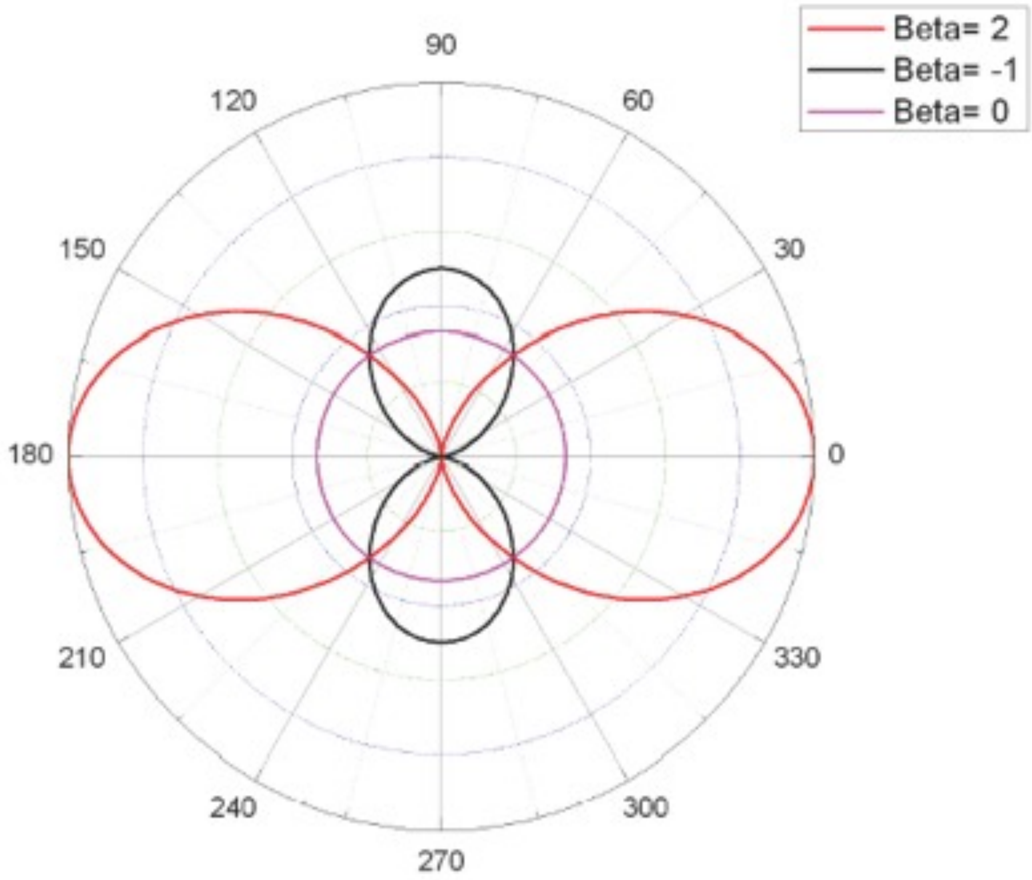


Fig. 4. Partial ion yield of different S clusters across the S 2p edge. All spectra have been scaled to the most intense one, S_2. The S 2p ionization energies at 170.5 (S $2p_{3/2}$) and 171.7 eV (S $2p_{1/2}$) [18] are included as vertical lines.

Inner shell photoionization of Sulphur clusters, created by laser ablation as a function of cluster size.

Advanced light source, Berkeley

Studies of simultaneous ionization/excitation of electrons in atoms



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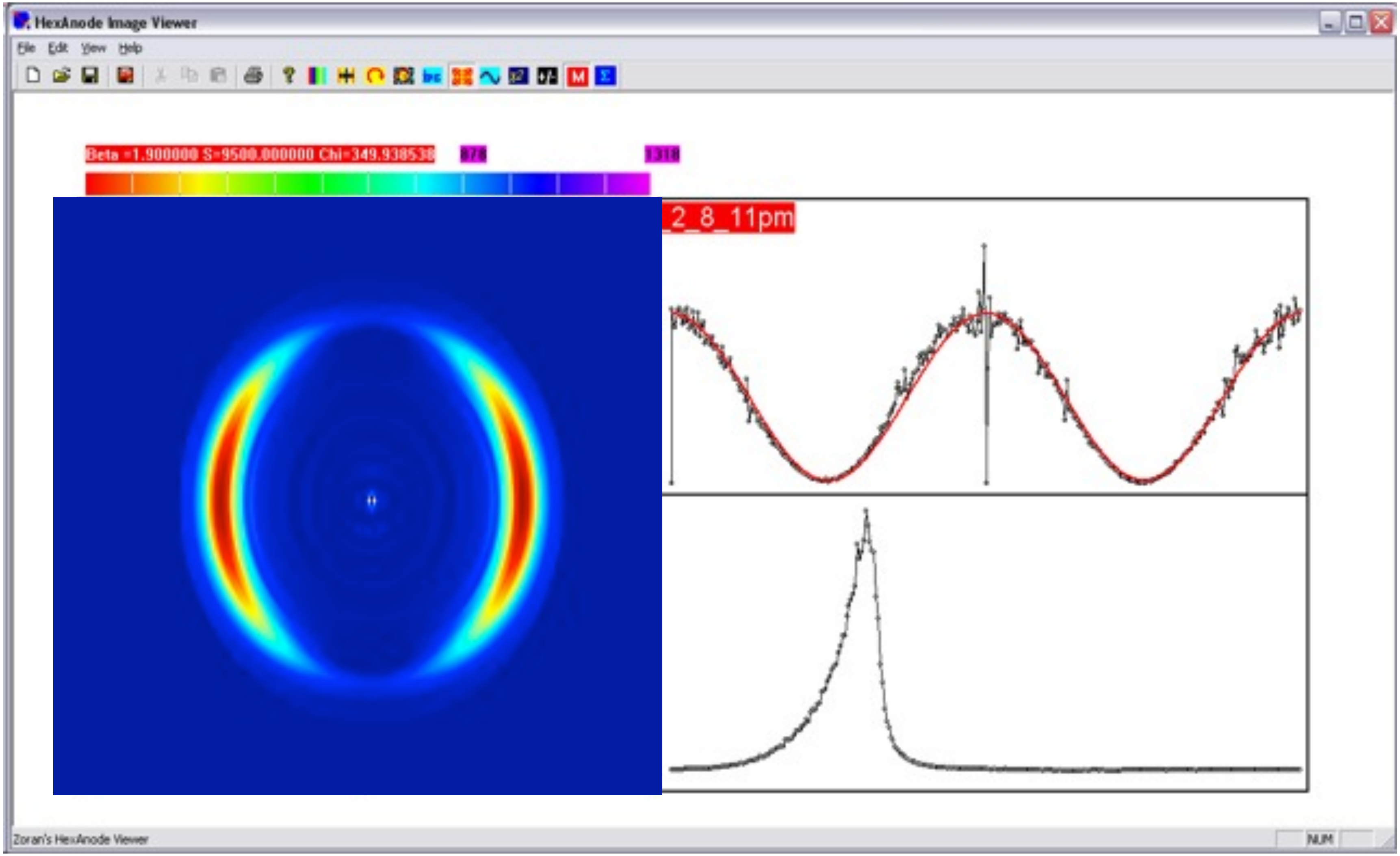

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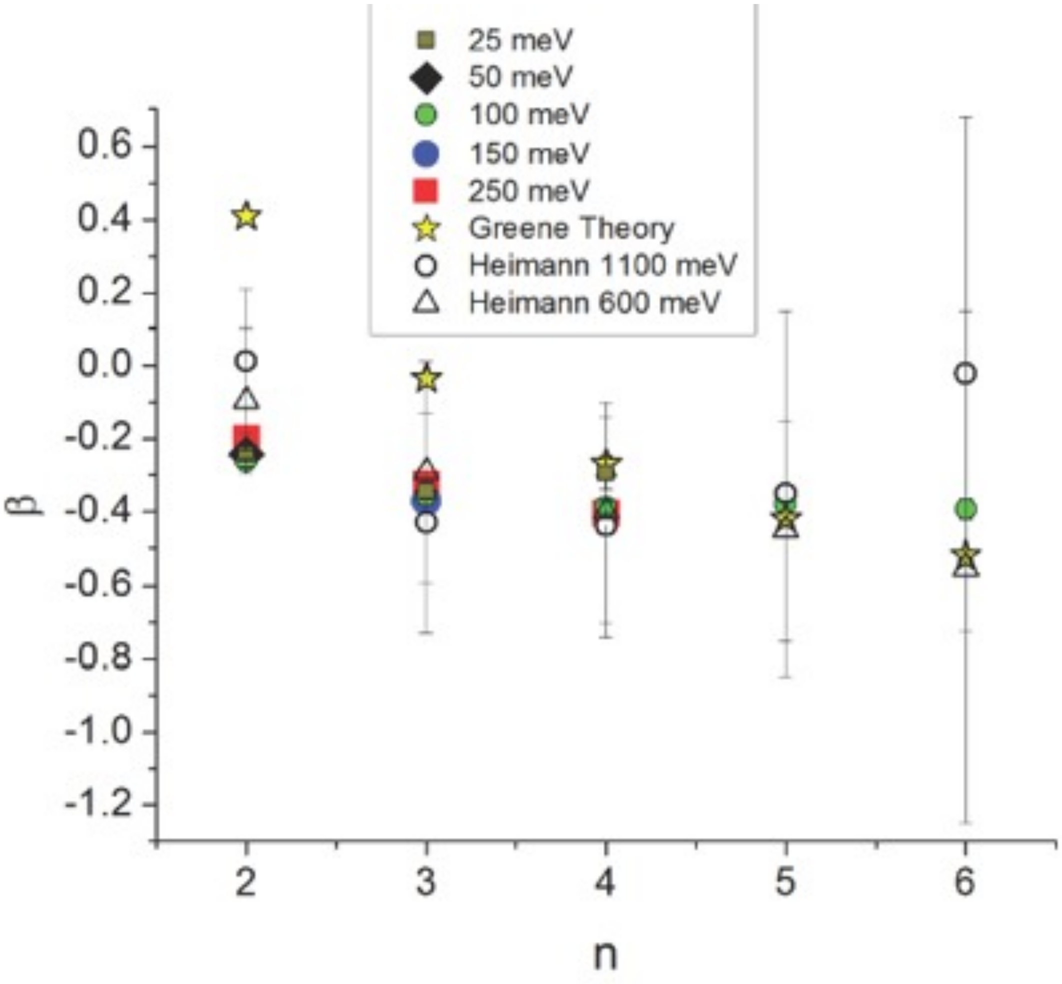
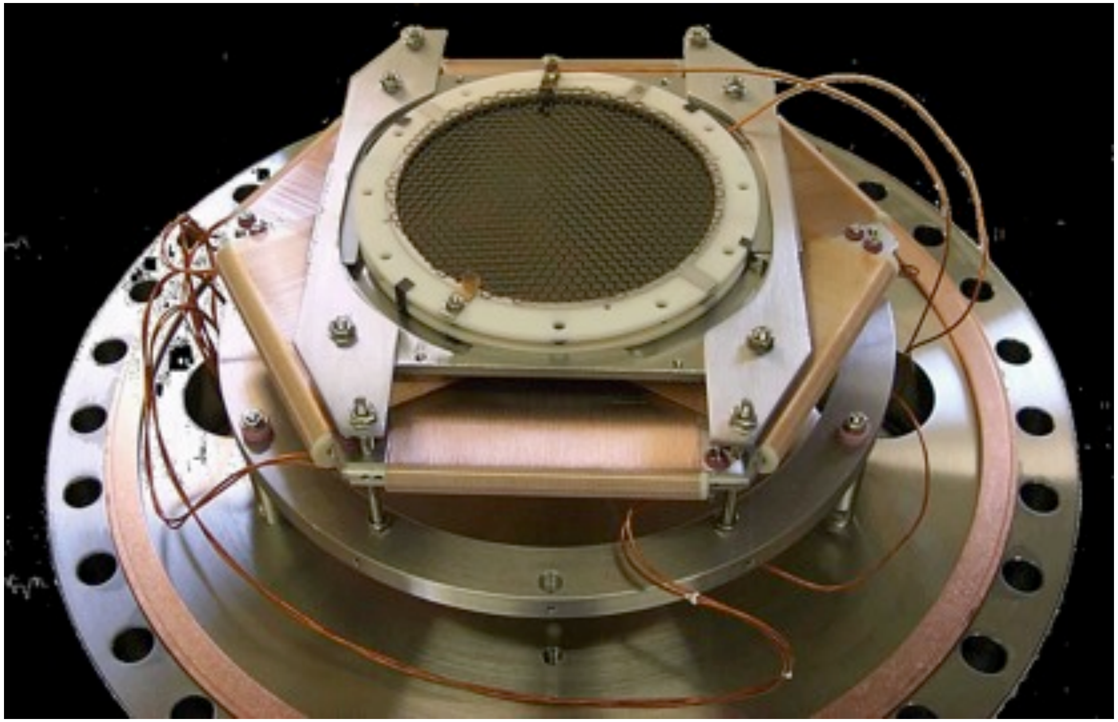


Made possible by position sensitive detectors And coincidence measurements



Final remarks

-Gasphase atomic and molecular studies in synchotrons can be useful tools to characterize and improve the performance of a beamline, besides its intrinsic interest.

-A synchrotron is made of several important parts. From the user´s stand point of view, the beamline can make the difference between a successful experiment.

-Good beamlines at second generation sources can produce good science

- The instrumentation available

-. Building and binding the comunity is a good –needed- step to take, before building the machine itself.

ALS, Berkeley

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elettra

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