

LABORATORIJA ZA FIZIKU ATOMSKIH SUDARA

# SEMINAR

TEMA: ELECTRON LOSS FROM NEGATIVE IONS IN COLLISIONS  
WITH ATOMS AND MOLECULES

VРЕМЕ: 20. APRIL 1990. 9:00

МЕСТО: СОБА 300

ПРЕДАВАЧ: DR VLADIMIR A. ESAULOV

LABORATOIRE DES COLLISIONS ATOMIQUES  
ET MOLECULAIRES  
UNIVERSITE PARIS-SUD ORSAY

# Electron detachment from negative ions in collisions with atoms & molecules

work done at:-

LAB. Collisions Atomiques + Moléculaires  
ORsay

Dept. of Physics, College of William + Mary  
Williamsburg, USA  
group of R. L. Champion

LAB. DE PHYSIQUE ET OPTIQUE  
CORPUSCULAIRE, Univ. PARIS 6  
PARIS

group of R. I. HALL

## OBJECTIVE

### STUDY OF IONISATION PHENOMENA

AT **LOW ENERGIES.**

→ MOLECULAR DESCRIPTION OF THE COLLISIONAL SYSTEM.

WHY NEGATIVE IONS?

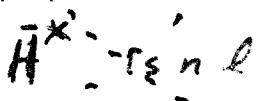
CHARACTERISTICS -

— LOW BINDING ENERGIES

$$H^- \approx 0.75 \text{ eV}$$

$$F^- \approx 3.4 \text{ eV}$$

— THEY HAVE NO "SINGLY EXCITED STATES." i.e.

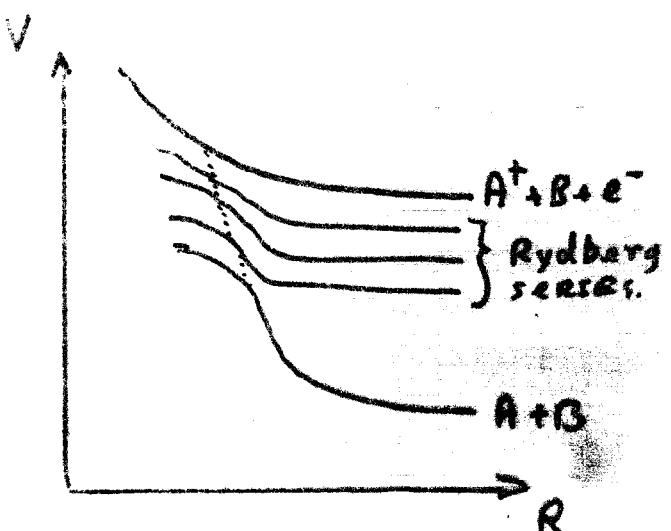


BUT ONLY

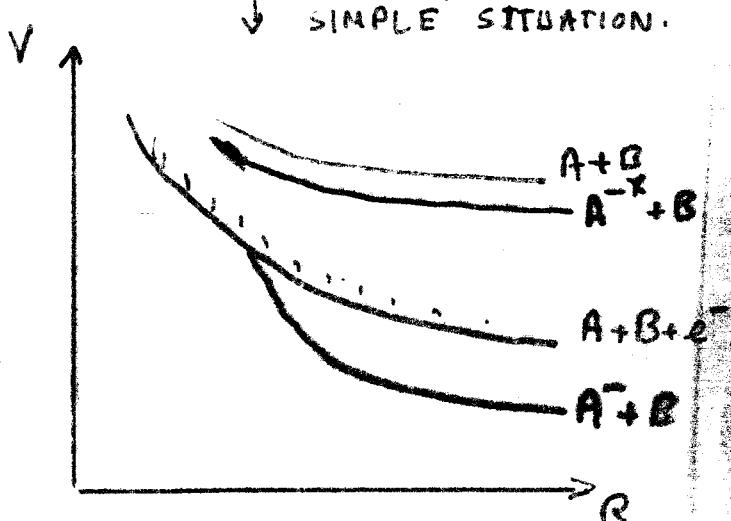


ATOM + ATOM

$A^- + \text{ATOM}$

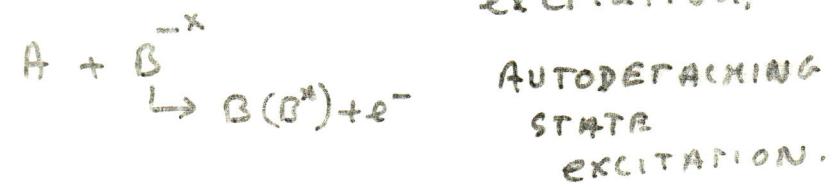


↓ "SIMPLE" SITUATION.



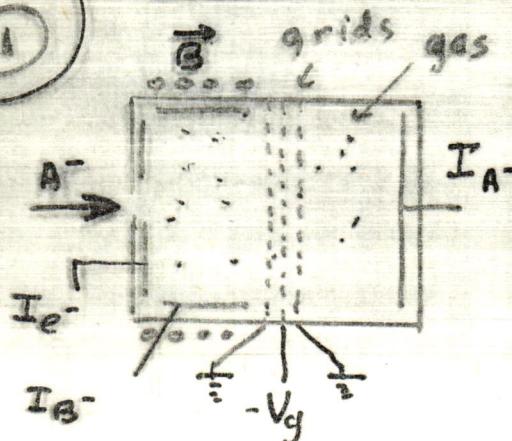
(3)

## TYPES OF REACTIONS



... etc.

## TYPES OF EXPERIMENTS.



TOTAL cross sections.  
(WILLIAMS BURE)



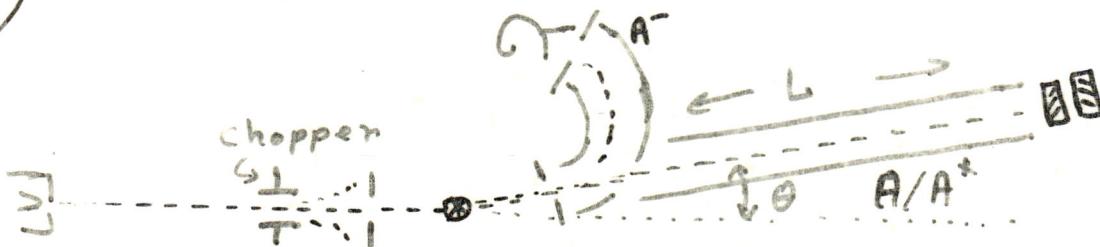
$I_{A^-}$ ,  $I_{e^-}$ ,  $I_{B^-}$ , Pressure

• GLOBAL INFORMATION, CROSS SECTION MAGNITUDE, THRESHOLDS. YOU CAN ALSO GET SOME IDEA OF THE DYNAMICS (VELOCITY DEPENDENCE) BY LOOKING AT ISOTOPIC EFFECTS

- $H^-/D^-$  + TARGET
- $A^- + H_2/D_2$



## ENERGY LOSS STUDIES (ORSAY).



ELECTROSTATIC ANALYSIS ( $A^-$ ), TIME OF FLIGHT (TOF) ENERGY LOSS MEASUREMENTS FOR ( $A$ ).

- ENERGY RANGE -  $100 \text{ eV} - 5 \text{ keV}$
- ANGULAR " -  $0 \div 30 \text{ deg}$

ENERGY RESOLUTION  $\approx 0.2 \text{ eV} \div 2 \text{ eV}$

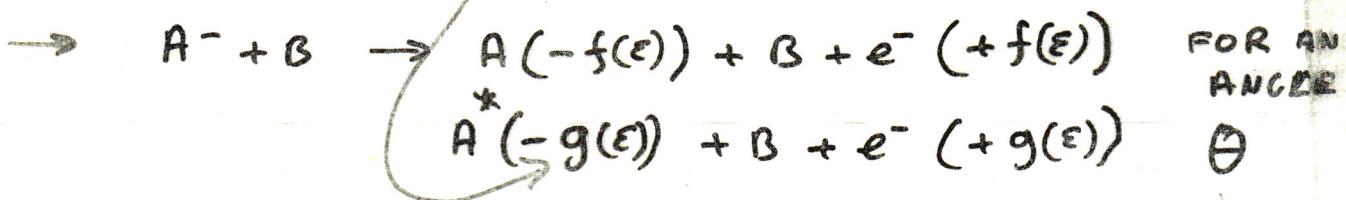
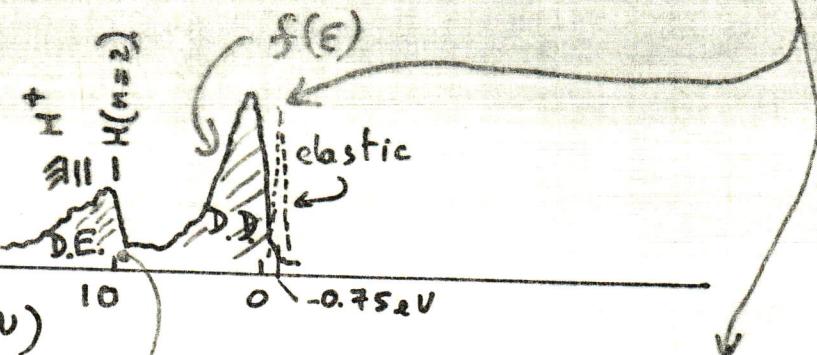
TOF LENGTH  $L = 0.5 \text{ m} \div 7.5 \text{ m}$

- ① → STUDY SEPARATELY DETACHMENT INTO GROUND & EXCITED STATES
- ② → DETERMINE DIFFERENTIAL CROSS SECTIONS WHICH GIVE INFORMATION ABOUT THE IMPORTANCE OF PROCESSES AS A FUNCTION OF INTER NUCLEAR SEPARATION.

## TOF (contd.)

- ③ GIVE INDICATIONS ABOUT THE SPECTRA OF  $e^-$  emitted AND THEIR IMPACT PARAMETER (ANGULAR) DEPENDENCE.

$H^- + He$   
 $750 \text{ eV}$   
 $\theta = 0.6^\circ$



ATOM SCATTERING ANGLE  $\leftrightarrow b$ , THE

$f(\epsilon)$  - is a sum over all  $e^-$  ejection angles.

TOF  $\rightarrow$  FAIRLY DETAILED INFORMATION,

- BUT — THE ENERGY RESOLUTION IS NOT GOOD
- DECAY CHANNELS FOR EXCITED STATES ARE NOT KNOWN
- COLLISION ENERGY RANGE IS FAIRLY HIGH  
 $E \geq 100 \text{ eV}$  (detection efficiency FOR NEUTRAL ATOMS).

## ③ ELECTRON SPECTROSCOPY

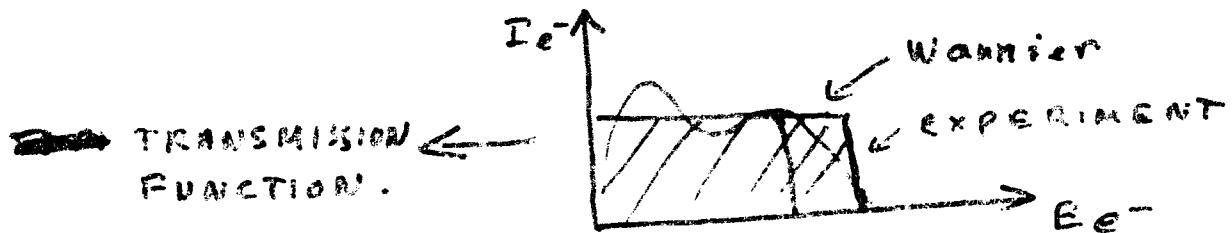
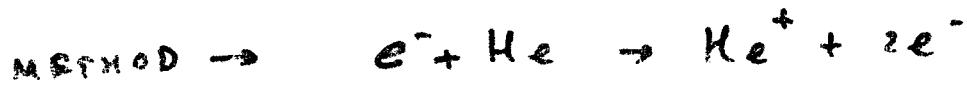


- A WITHOUT COINCIDENCES.  
 ② ELECTRON SPECTRUM SUMMED OVER IMPACT PARAMETERS  
 BUT CORRESPONDS TO A GIVEN  $e^-$  ejection angle.

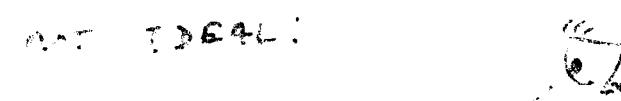
- ② GET INFORMATION PRODUCED AND ABOUT EXCITED STATES THEIR DECAY CHANNELS.

(6) ELECTRON SPECTROSCOPY (CONTD.).

PROBLEMS :- TRANSMISSION FUNCTION OF THE ANALYSER + OPTICS.



THIS IS NOT IDEAL:



THE COLLISION VOLUME MAY NOT BE THE SAME.

A BETTER WAY WOULD BE TO DO A  $e^-$  TIME OF FLIGHT SPECTRUM — NOT DONE EXTENSIVELY.

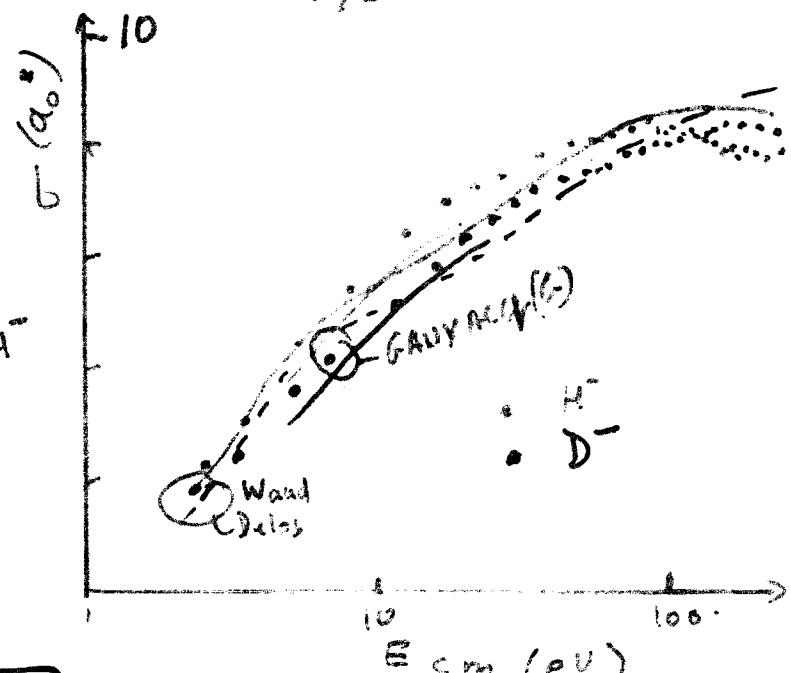
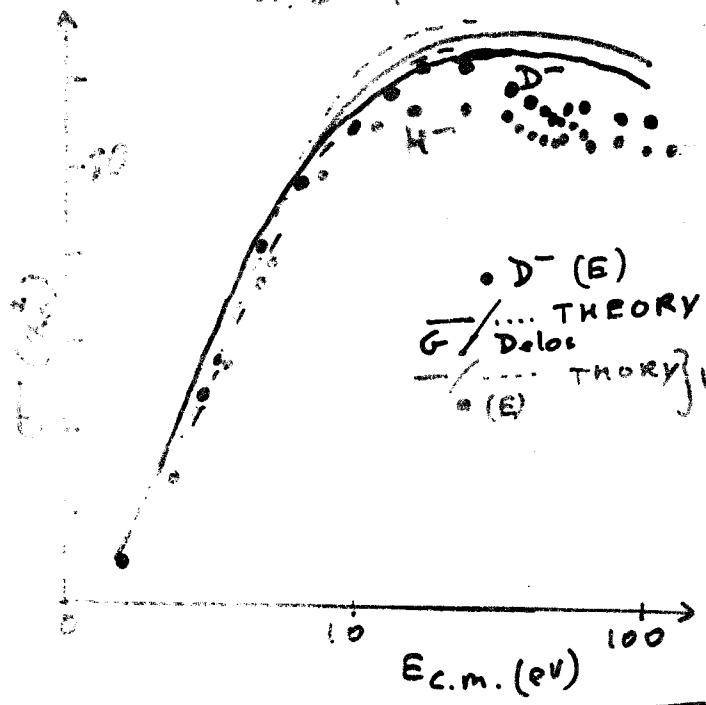
EXCEPTION —  $H + He$  — some scattering angles of H.  $\rightarrow$  Linder (Kaiserslauter)

## RESULTS

SYSTEMS STUDIED -  $H^-$ ,  $F^-$ ,  $Cl^-$ , ... }  $He, Ne, ...$   
 $O^-$ ,  $S^-$ , ... }  $Na, Li, ...$   
 $Li^+, Na^+$ , ... }  $H_2, Ne, D_2$

HERE WE SHALL MAINLY LOOK AT  $H^-$ .

### ① TOTAL CROSS SECTIONS.



N.B.

$$\sigma_{H^-} < \sigma_{D^-}$$

STEEP RISE OF  $\sigma$

TWO DIFFERENT

BEHAVIOR!!!

$$\sigma_{H^-} > \sigma_{D^-}$$

SLOW RISE OF  $\sigma$

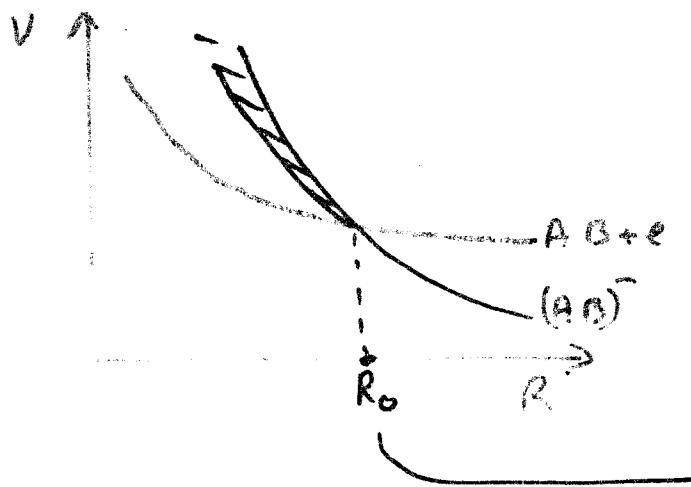
THE PLOT  $\sigma(E_{c.m.}) \rightarrow$  FOR THE SAME CENTER OF MASS (C.m.) ENERGY ( $E_{cm}$ ) THE IONS FOLLOW THE SAME TRAJECTORY (SAME DISTANCE OF CLOSEST APPROACH) BUT THE RADIAL VELOCITIES ARE DIFFERENT. AND THE TIME A SYSTEM SPENDS IN THE INTERACTION REGION IS DIFFERENT.

①  $H^-D^- + He \rightarrow$  THE SLOWER  $D^-$  HAS A BIGGER  $\sigma$

## GOOD OLD DESCRIPTIONS.

LOCAL COMPLEX POTENTIAL MODEL.  
(RESONANT STATES).

STATIC DESCRIPTION



$$V(R) = E(R) - i \frac{\Gamma(R)}{2}$$

$\Gamma(R)$  - width,  
which depends  
only on  $R$ , but  
not on velocity

$$\Gamma(R) = 0 \text{ FOR } R > R_0$$

— Detachment probability

$$P_d = 1 - \exp(-\Gamma dt)$$

$$= 1 - \exp\left(-\int_{R_{\min}}^{\infty} dR \frac{\Gamma(R)}{v_R}\right), \quad v_R \text{ - radial velocity}$$

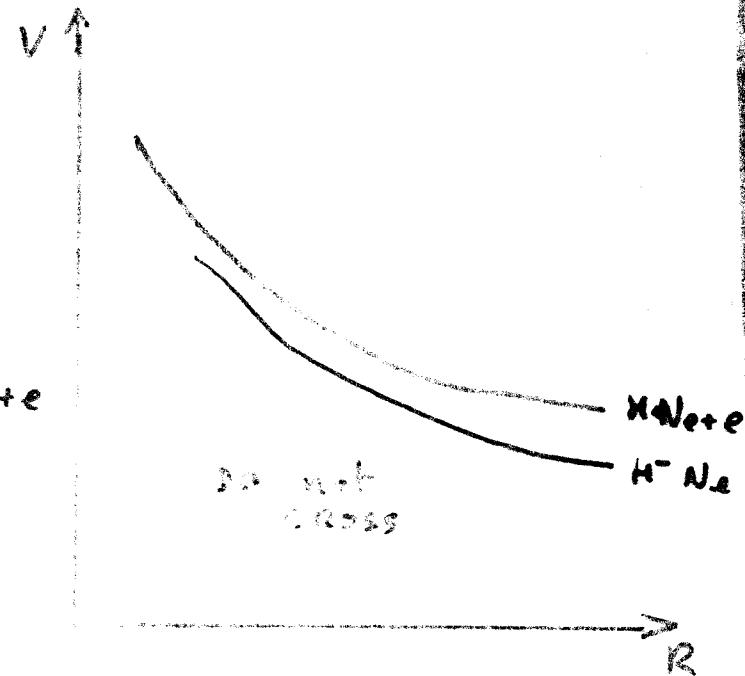
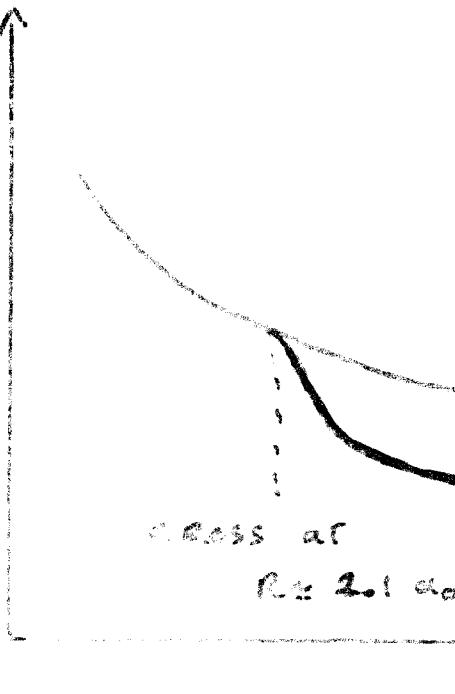
$R_{\min}$  - distance of closest approach.

— Predictions :- FOR  $H^-/D^-$  - THE SLOWER ISOTOPE WILL SPEND A LONGER TIME IN THE CONTINUUM AND  $\sigma_{D^-} > \sigma_{H^-}$ .

THIS SEEMS OK FOR  $H^- + He$  BUT IS NOT OK FOR  $H^- + Ne$ .

THERE EXIST MANY OTHER EXAMPLES WHERE THESE PREDICTIONS FAIL AND WHERE OBVIOUSLY COLLISION VELOCITY DEPENDENT EFFECTS (INCREASE OF σ WITH INCREASING VELOCITY) ARE OBSERVED.

(10)

 $H^- + He$ SCHERAFIKI  
(SCHEMATIC) $H^- + Ne$ 

LEGACY OF THE SCHEMATIC POTENTIALS  
DOES NOT COMPARE WITH THE  
LOCAL MOMENT POTENTIALS FOR IONIZATION.

ONE NEEDS OTHER DESCRIPTIONS WHERE  
DYNAMIC EFFECTS ARE TAKEN INTO ACCOUNT.

① NON-LOCAL RESONANT STATE FORMALISMS.

W. DOMCKE - FRG

J. DELOS - WILLIAMS BURG

② EFFECTIVE RANGE DESCRIPTIONS

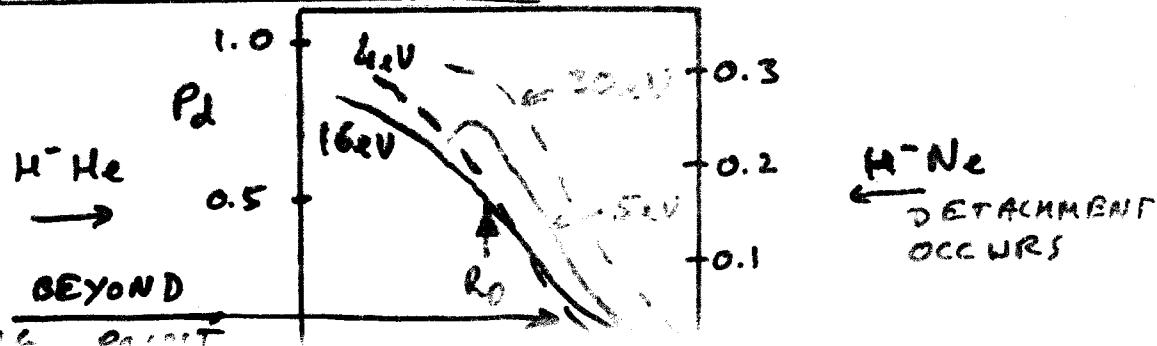
- "ZERO RANGE POTENTIAL MODEL"  
(ZRP.) DEM'KOV - LENINGRAD

- GAYDAG - ORSAY

EXAMPLE.

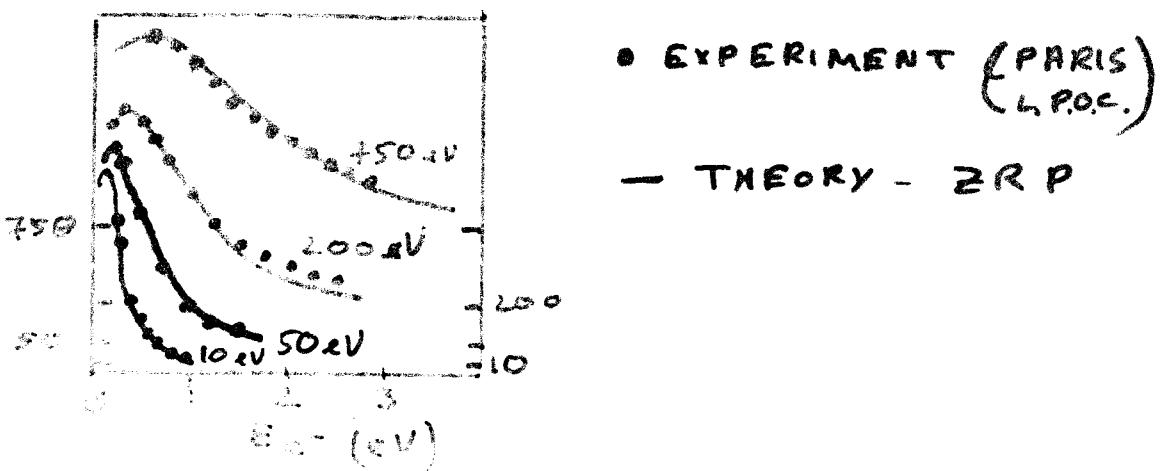
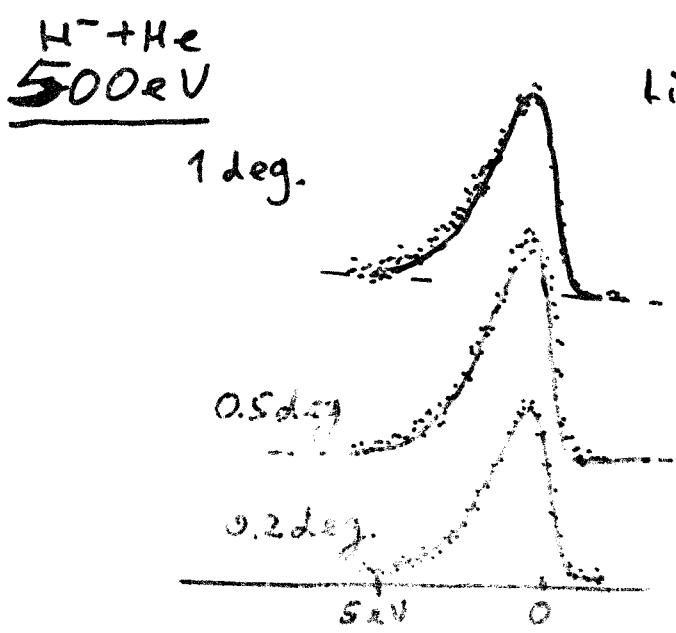
ZRP

TRANSITIONS BEYOND THE



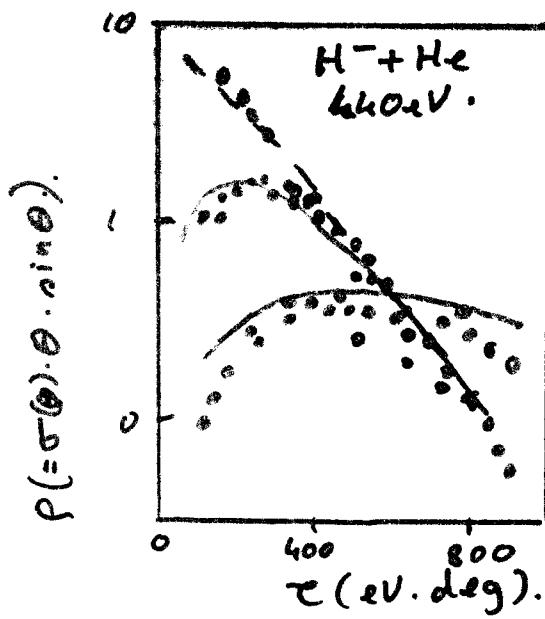
APPLICATIONS.② TOTAL CROSS SECTIONS —  
(GOOD AGREEMENT).

③ ELECTRON SPECTRA [ SUM OVER IMPACT PARAMETERS ].

④ Electron spectra - IMPACT PARAMETERS DEPENDENCE  
TOF = 1000 fmLine-Theory ZRP  
• - EXPERIMENT.THESE ARE NEUTRAL  
H atom TOF  
SPECTRATHEORY IS A  
CONVOLUTION FOR  
EJECTION KINEMATICS  
+ APPARATUS EFFECTS -  
( $\Delta E = 0.5 \text{ eV}$ )

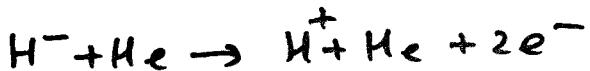
THERE EXIST SOME RECENT  $e^- \leftrightarrow H$   
COINCIDENCE MEASUREMENTS BY TOF OF  $e^-$   
— LINDNER (Kaisers Lautern). THESE DATA  
ALSO AGREE WITH THE ZRP  
CALCULATIONS.

④ - Differential cross sections TOF - ORSAY.

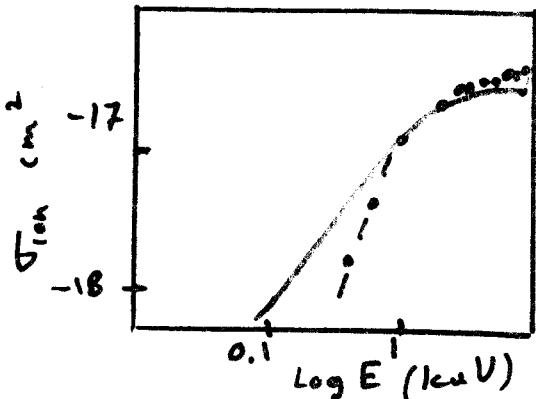


ZRP does not take into account excitation processes.  
THESE WERE TAKEN INTO ACCOUNT IN A "hybrid" model.  
assuming the outer H- electron and the core (H+He) collision evolve independently.

⑤ Ionisation



ZRP  
"hybrid"



• EXPERIMENT  
= THEORY  
USING  
DIFFERENT  
SETS OF  
EXPERIMENTAL  
(H+He) data.

CONCLUSION

A GOOD DESCRIPTION OF ELECTRON DETACHMENT IS OBTAINED WHEN DYNAMIC EFFECTS (NUCLEAR VELOCITY) ARE TAKEN INTO ACCOUNT.

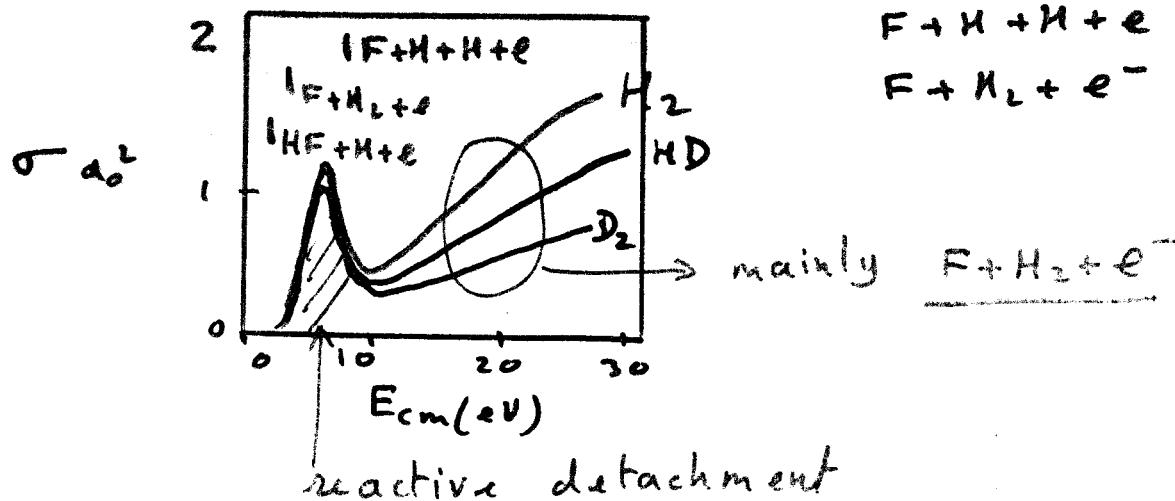
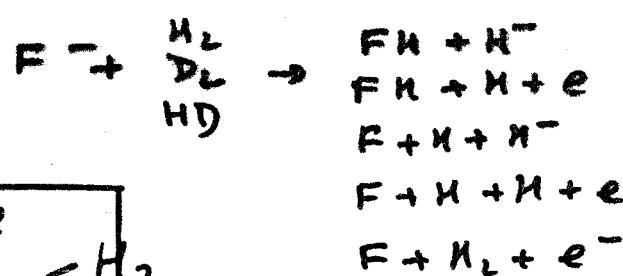
THIS IS NOT THE CASE OF LOCAL RESONANT STATE DESCRIPTIONS.

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# COLLISIONS WITH MOLECULES

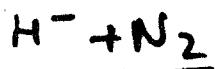
THERE ALSO EXIST DYNAMIC EFFECTS:-

EXAMPLE :-



THESE CROSS SECTIONS ARE DIFFERENT FOR THE SAME CENTER OF MASS ENERGY BUT ARE THE SAME FOR THE SAME LAB. ENERGY i.e. FOR THE SAME COLLISION VELOCITY.

## OTHER PROCESSES.



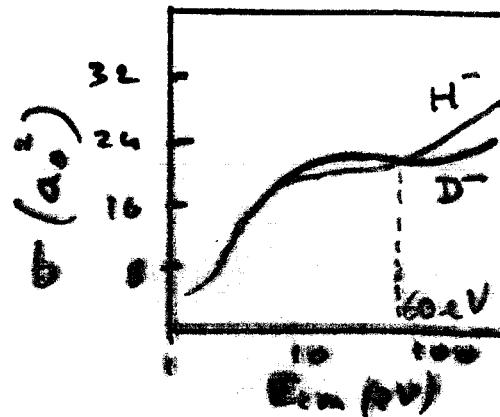
$$E < 60 \text{ eV}$$

$$\sigma_{H^-} < \sigma_{D^-}$$

$$\text{but } E > 60 \text{ eV}$$

$$\sigma_{H^-} > \sigma_{D^-}$$

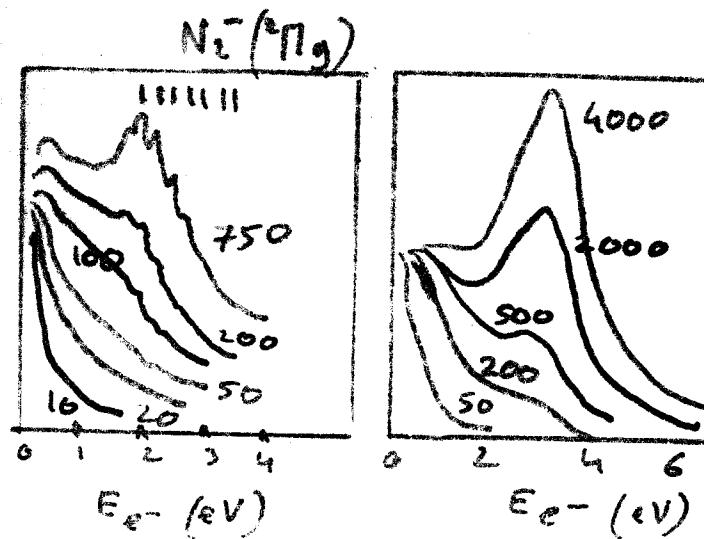
## TOTAL CROSS SECTION



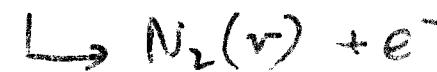
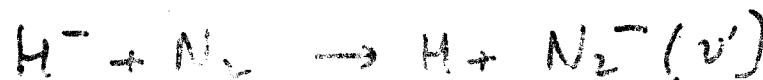
ONSET OF SOMETHING ?

(14)

# ELECTRON SPECTRA

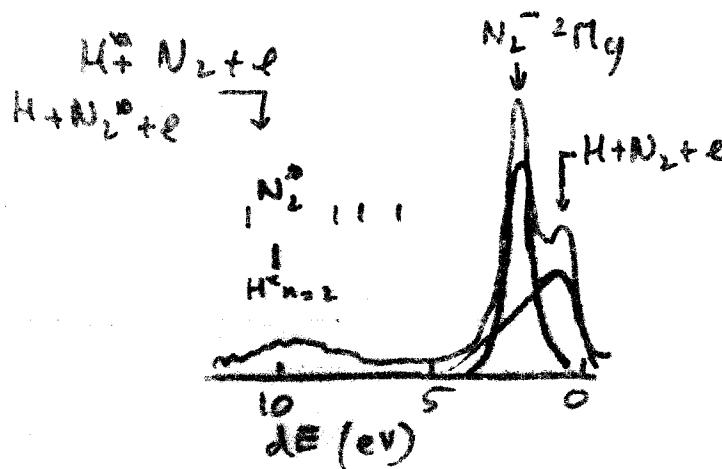


AT ABOUT 50-eV ONE SEES THE APPEARANCE OF STRUCTURES DUE TO THE DECAY OF  $N_2^- \text{ } ^2\text{P}_g$  RESONANCE.

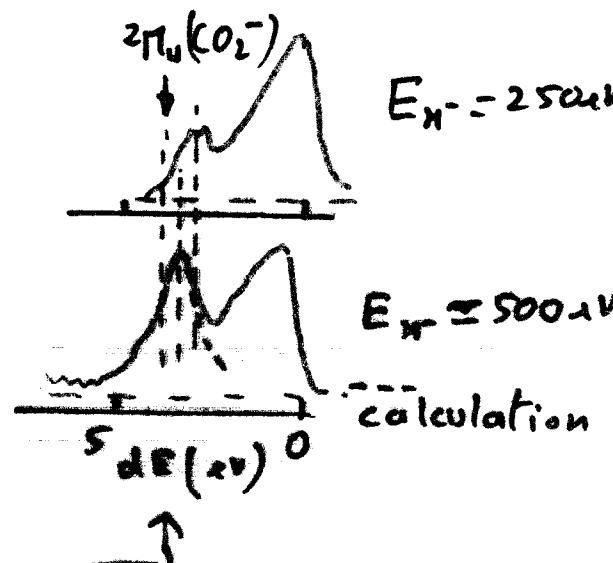


THIS MUST BE POSSIBLE FOR THE CHANGE IN THE ISOTOPE EFFECT.

## TOF (H atom) spectra



FRANCK KONDON POSITION



THE PEAK LIES BELOW THE FRANCK KONDON RESONANCE POSITION AT LOW COLLISION ENERGIES. STRANGE

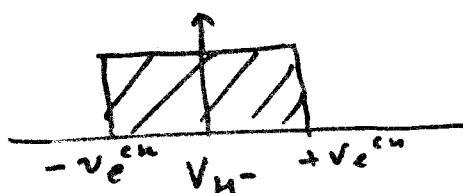
15  
CONSIDER FAST COLLISIONS OF  $H^-$



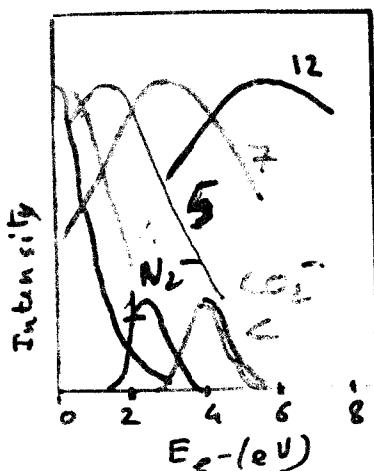
BINARY COLLISION APPROXIMATION.

CONSIDER THE SCATTERING OF THE OUTER  $e^-$  ON THE TARGET

$$\vec{v}_e^{\text{lab}} = \vec{v}_{H^-} + \vec{v}_e^{\text{cm}}$$



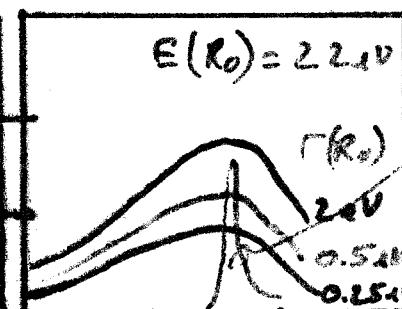
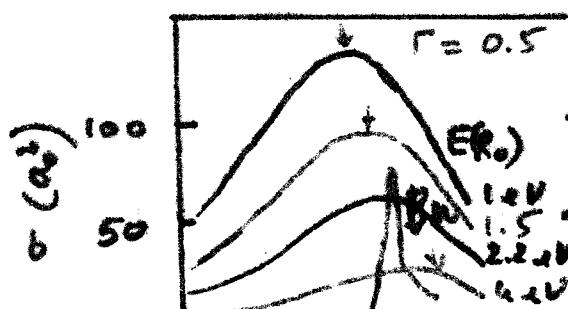
velocity distribution schematic



Energy distribution in the electron wave packet (calculated - Gaugap-Hergenborg) for different  $H^-$  energies.

-Frank Condon envelope for the  $N_2^-$  and  $CO_2^-$  resonances.

For low collision energies the translational energy of the electron is not high enough and only the low energy tail of the ~~resonance~~ resonance is excited. At high energies the  $e^-$  energy is high enough so that the F.C. position is attained in the TOF spectra.



$e^-$  scattering cross section (Bret Wigner)

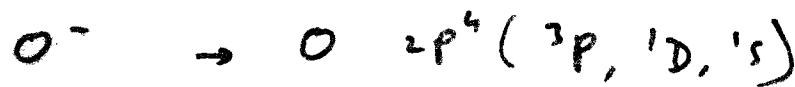
CROSS SECTION MAXIMUM REACHED  $E_e$  (eV)

BROADER RESONANCE

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## Two $e^-$ LOSS IN NEGATIVE ION COLLISIONS

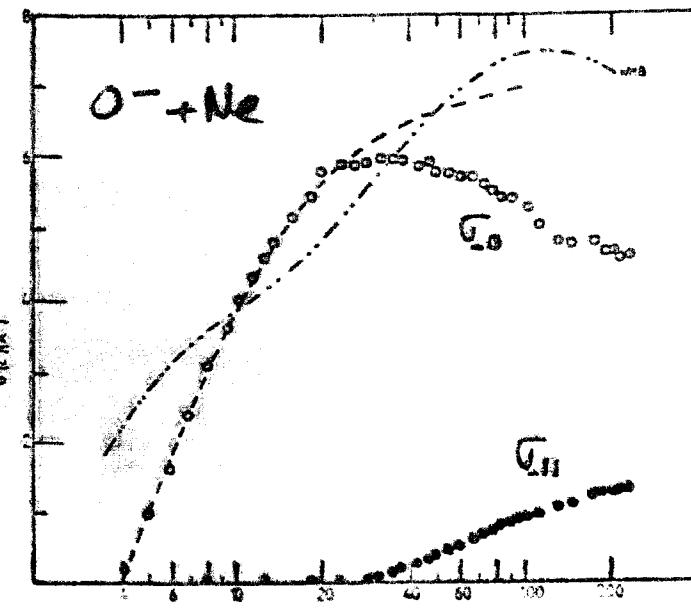
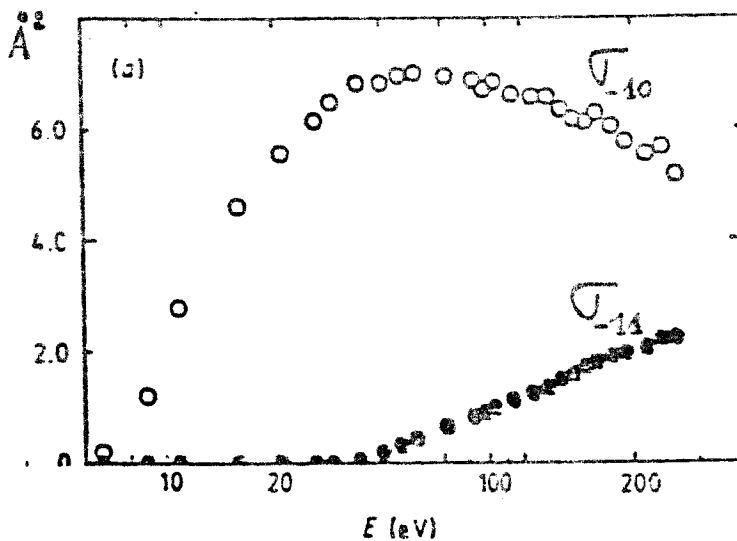
CASE OF OPEN SHELL PARENT ATOMS.



TOTAL AND DIFFERENTIAL CROSS SECTION MEASUREMENTS SHOW THAT IN SOME CASES THE TWO  $e^-$  LOSS CROSS SECTION MAY BE VERY LARGE AND ONSETS AT LOW ENERGIES.

F-/Ne

MECHANISM?

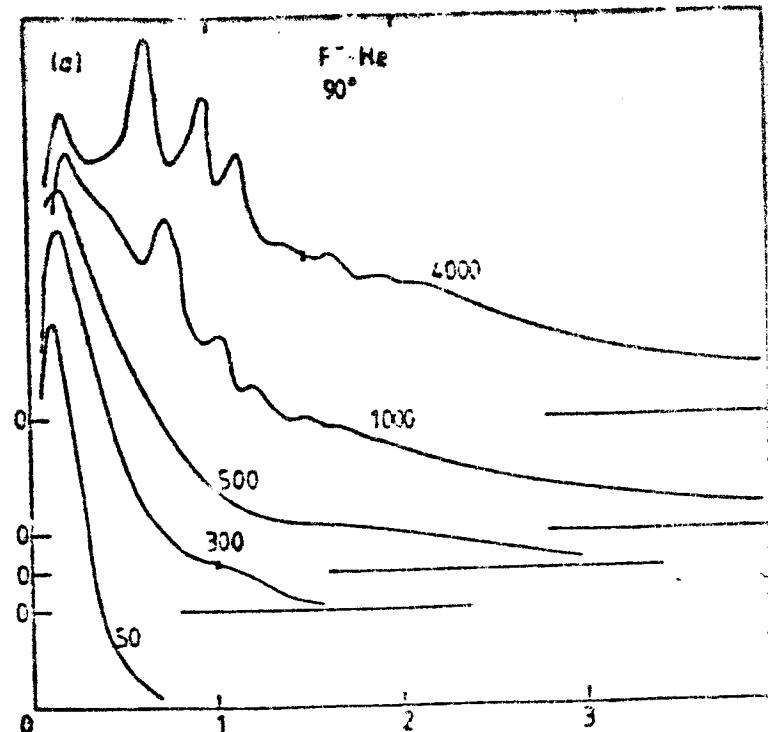
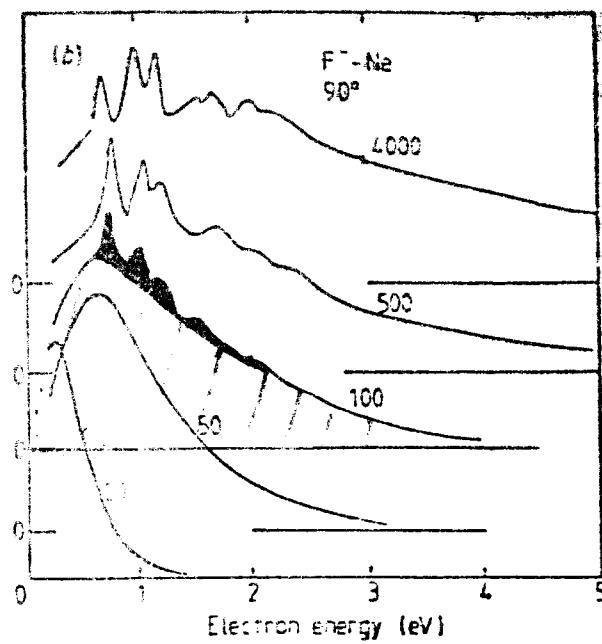


(17)

# ELECTRON SPECTRA.

→ PEAKS THAT  
ARE DUE TO

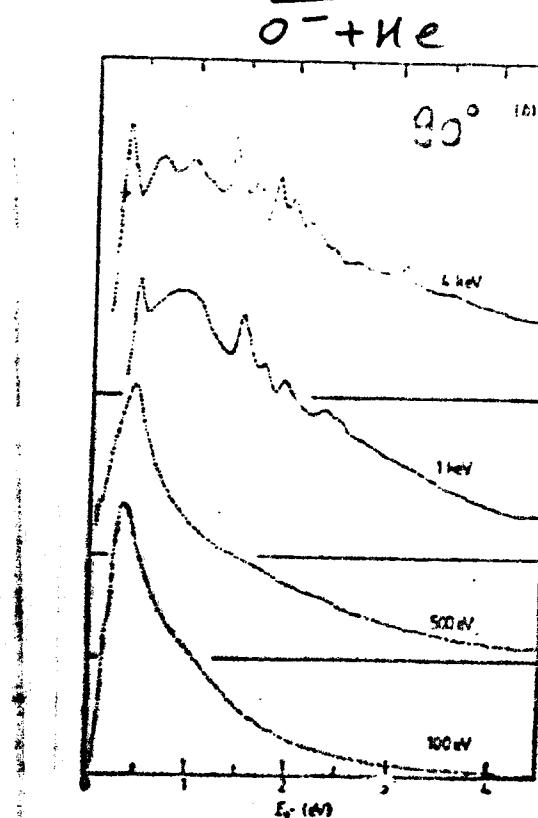
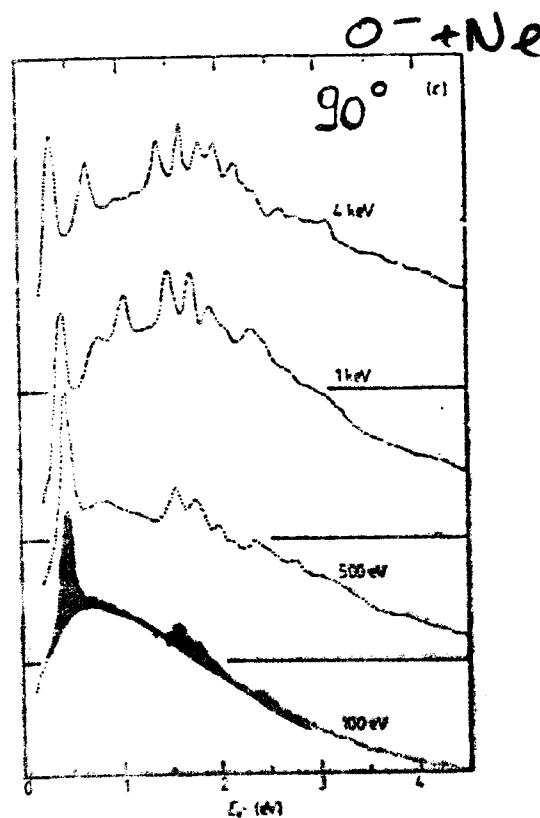
AUTOIONISING STATES.



THRESHOLDS  $F^- + Ne \sim 50 \text{ eV cm.}$

$$\frac{\sigma_{-11}}{\sigma_{-10}} \approx 3\% \text{ PEAK AREAS}$$

$$\frac{\sigma_{-11}}{\sigma_{-10}} = 4\% \text{ TOTAL CROSS SECTION}$$



TRANSITION AT THRESHOLD PROBABLY DUE  
TO AUTIONISING STATE

(1B)  $F^+(s)$  stabilized

$$F^+(D) \underset{\text{closed}}{\overset{f^{-1}(3d)}{=}} = F(S^{n+e})$$

$$F^+(3P) \quad \frac{cccccc}{\equiv nl} = 3P^+ \quad F(3nl)$$

$$f \rightarrow f^{\ast}.$$

*F. C. P. G.*

## VALENCE

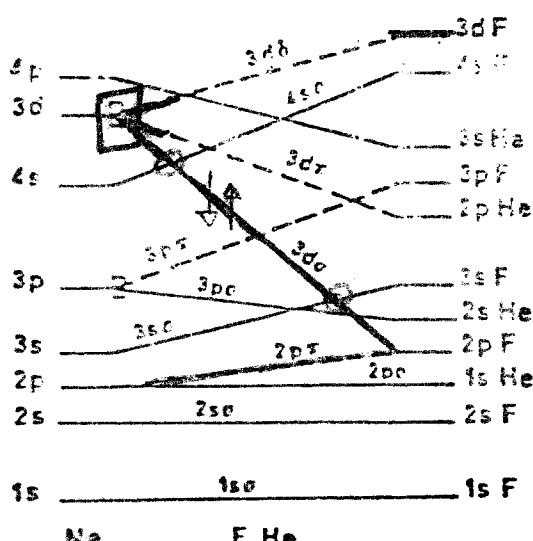
## AUTOIONISING STATES DUE TO

## THE EXISTENCE OF SEVERAL STATES

OF THE GROUND

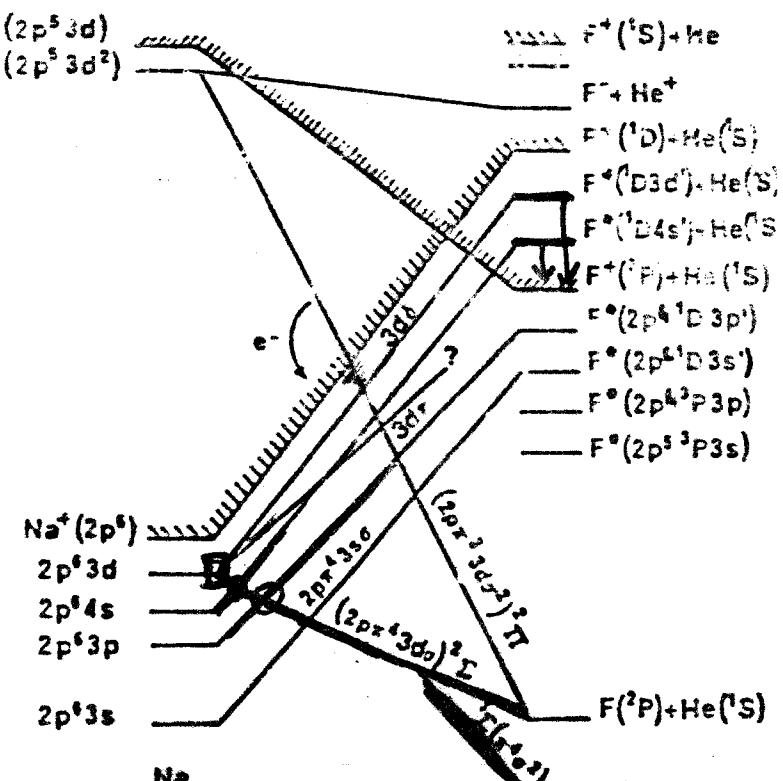
## PARENT ION CONFIGURATION

F + H<sub>2</sub>



### Diagramme de corrélation des orbitales

#### Mitral valve orbital calcification



### Diagramme de corrélation des États

## Molecular state correlations

step 1  $F^- He \rightarrow ^1\Sigma^+ \pi^+ e^- \xrightarrow[\text{electron}]{\text{REMOVE ONE}} ^3\Sigma^+ \pi^+ F K$

Excitation :- RADICAL COUPLING       $3d\sigma - 3s\sigma, 4s\sigma$   
 ROTATIONAL      "       $3d\sigma - 3d\pi - 3d\delta$

RESULT  $\rightarrow$   ${}^2\Sigma(\pi^4\sigma) \rightarrow \pi^4 n\lambda$  eg.  $\bullet 3d\pi^4 3d\delta$   
 $\downarrow$   $\downarrow$   $(1^1D) 2d^1$

MULTIPARAMETRIC STUDY  
OF ION - SURFACE  
COLLISIONS.

SIMULTANEOUS MEASUREMENTS

OF  $e^-$  SPECTRA

ION SPECTRA

$h\nu$  (visible) spectra

ALSO TOF SCATTERING

AND RECOLLING  
SPECTRA.

ANALYSIS:

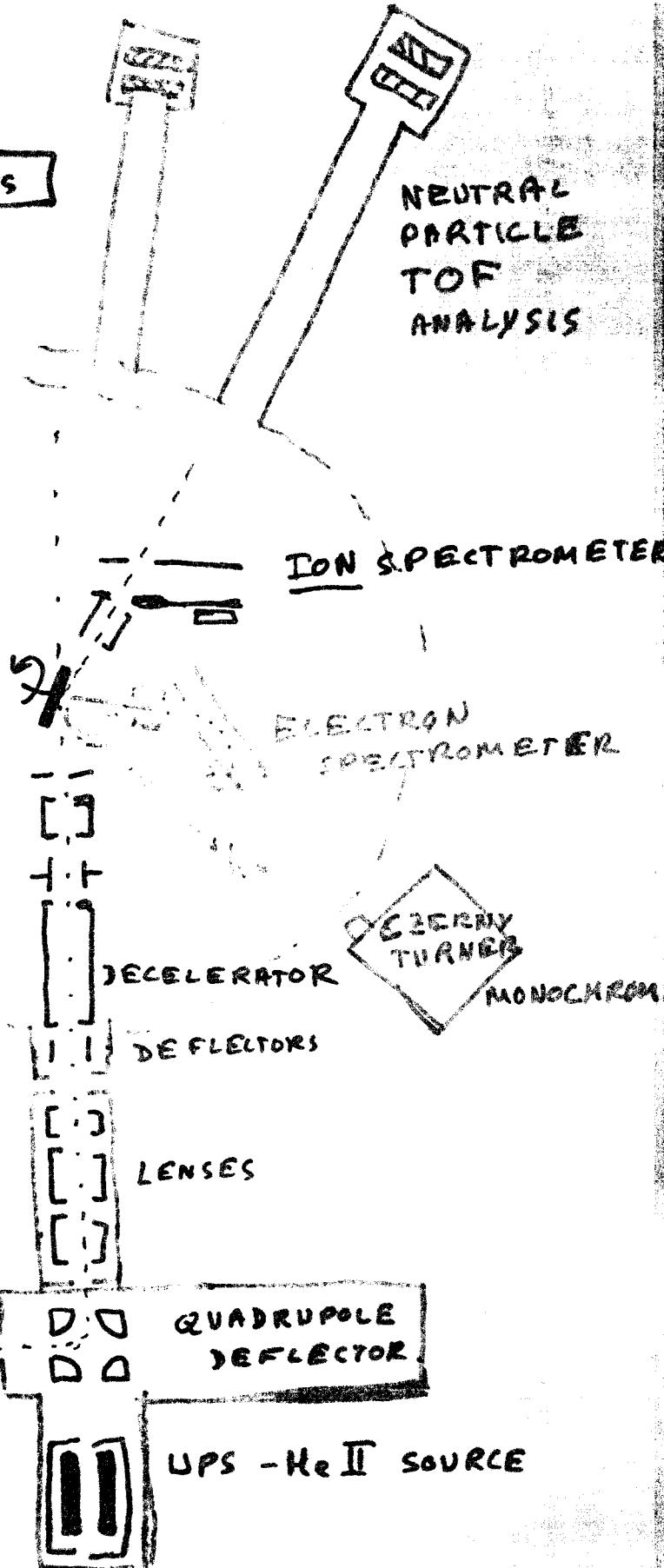
- 1) AES
- 2) UPS
- 3) TOF RECOLL.

BEAM LINE

LENS

$e^-$ -GUN  
AUGER  
SPEC.

$Ar^+$   
SPUTTER  
GUN



# FUTURE PROSPECTS:- (OKAY - )

ION

SCATTERING AT SURFACES.

(EE 51V ± 5KV)

OBJECTIVES. (1) STUDY OF RELATIVE ROLES OF ONE (RESONANT) AND TWO (AUGER) ELECTRON NEUTRALISATION.

- (2) STUDY OF THE ROLE OF COLLISIONS AT VERY CLOSE INTERNUCLEAR SEPARATION WITH SURFACE ATOMS. - EXCITED STATE PRODUCTION AND IONISATION
- (3) INTERACTIONS OF LOW ENERGY ION BEAMS WITH SURFACES WITH CHEMISORBED GASES. REACTIONS AND EXCITED STATE PRODUCTION.
- (4) INTERACTIONS OF MOLECULAR SPECIES WITH SURFACES. DISSOCIATION ETC.

## APPLICATIONS.

- i) MONITORING REACTION KINETICS
- ii) DETERMINATION OF ADSORPTION SITES AND BINDING ENERGIES OF ADSORBATES
- iii) MAKING OF THIN FILMS BY ION IMPLANTATION (e.g. DIAMOND FILMS FROM  $C^+$  BEAMS)
- iv) STUDIES OF INTERACTIONS OF LOW ENERGY BEAMS WITH SURFACES IN SPACE TECHNOLOGY :- PROBLEMS OF EROSION AND SPURIOUS LIGHT EMISSION (SHUTTLE GLOW PHENOMENA).