INTERNATIONAL ATOMIC ENERGY AGENCY
UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION

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COLLEGE ON ATOMIC AND MOLECULAR PHYSICS: PHOTON ASSISTED COLLISIONS IN ATOMS AND MOLECULES

(30 January - 24 February 1989)

Molecular Interactions from Scattering Experiments

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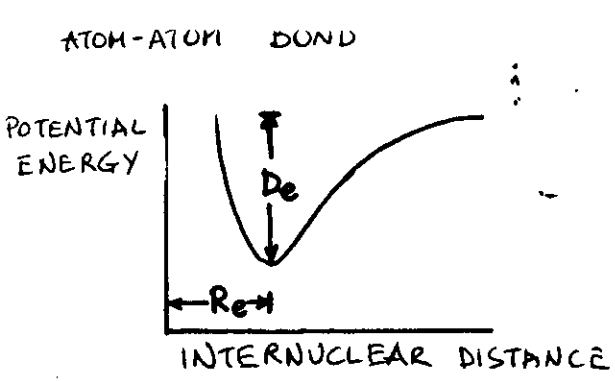
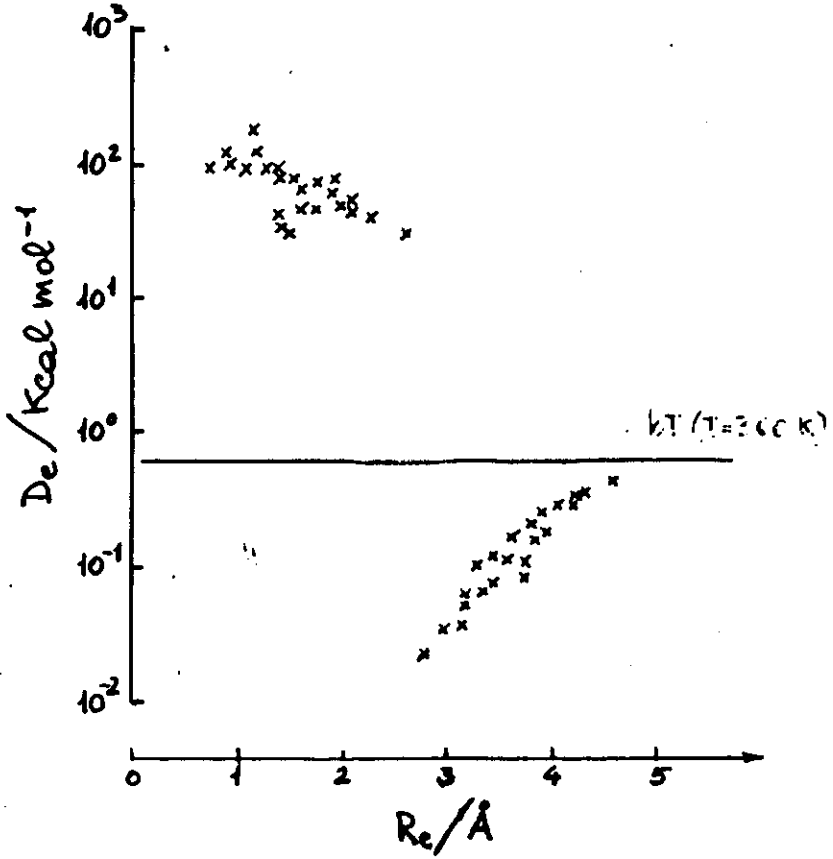




GASEOUS PROPERTIES

Equation of State

$$\frac{PV}{nRT} = 1 + \frac{B(T)}{T} + \frac{C(T)}{T^2} + \dots$$

(Virial Equation of State)

Transport Properties

Diffusion, $D(T)$

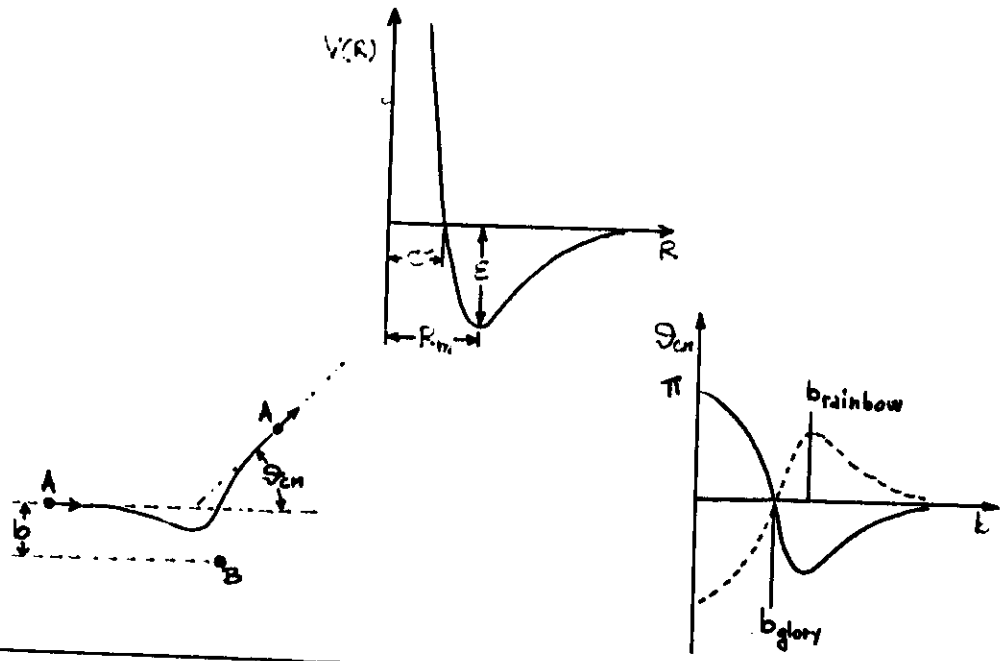
Viscosity, $\eta(T)$

Thermal Conductivity, $\lambda(T)$

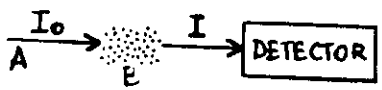
....

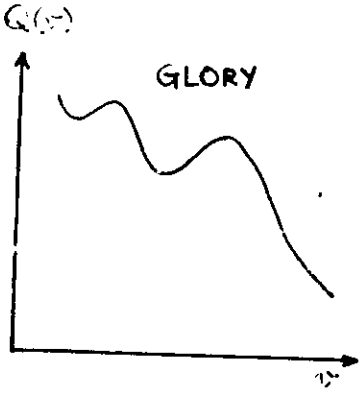
....

ELASTIC SCATTERING

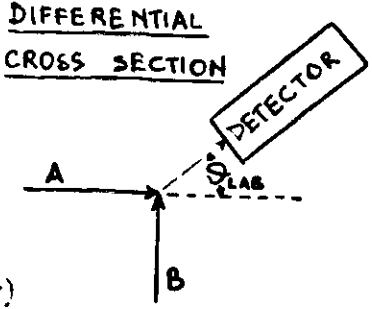


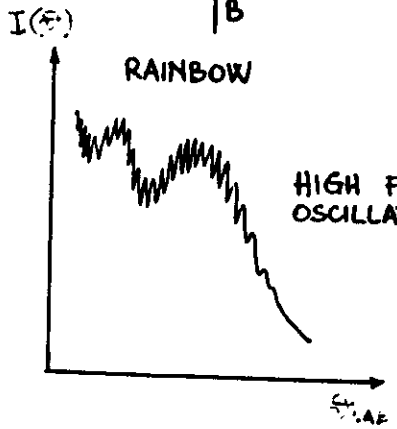
INTEGRAL CROSS SECTION



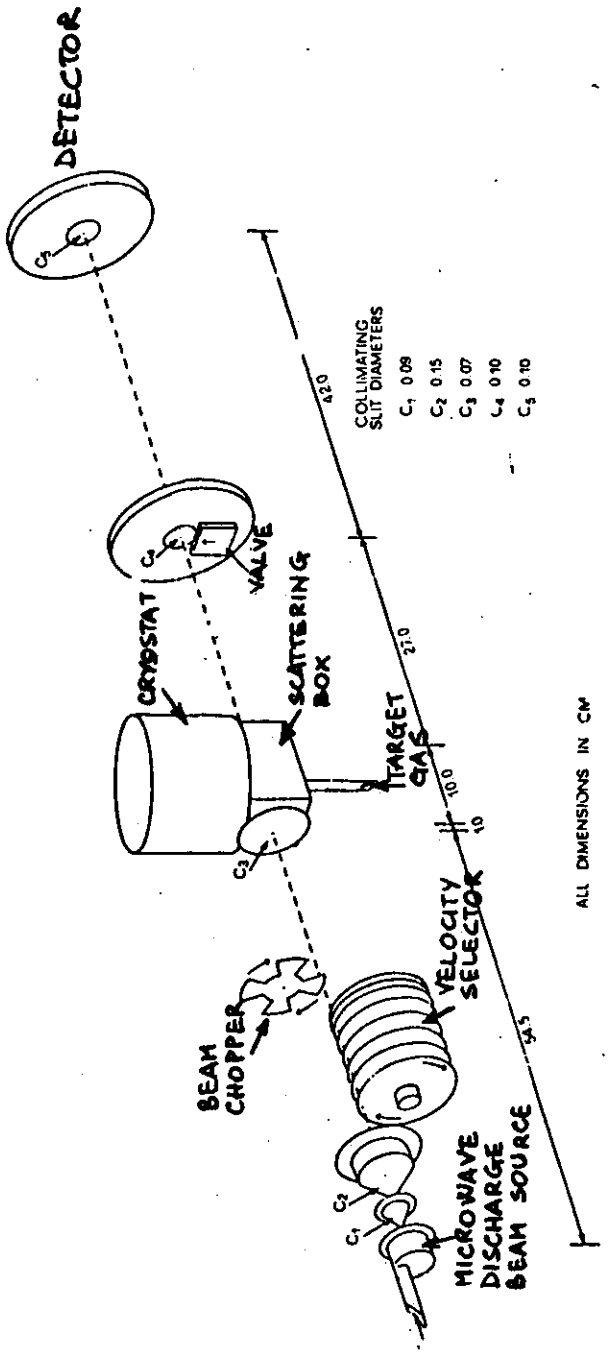


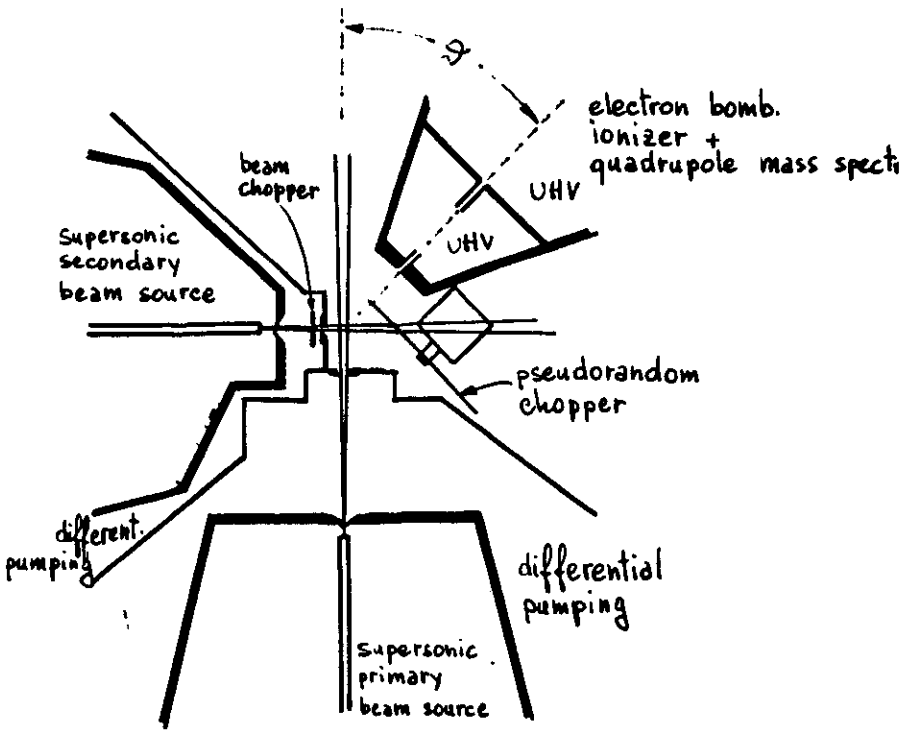
DIFFERENTIAL CROSS SECTION



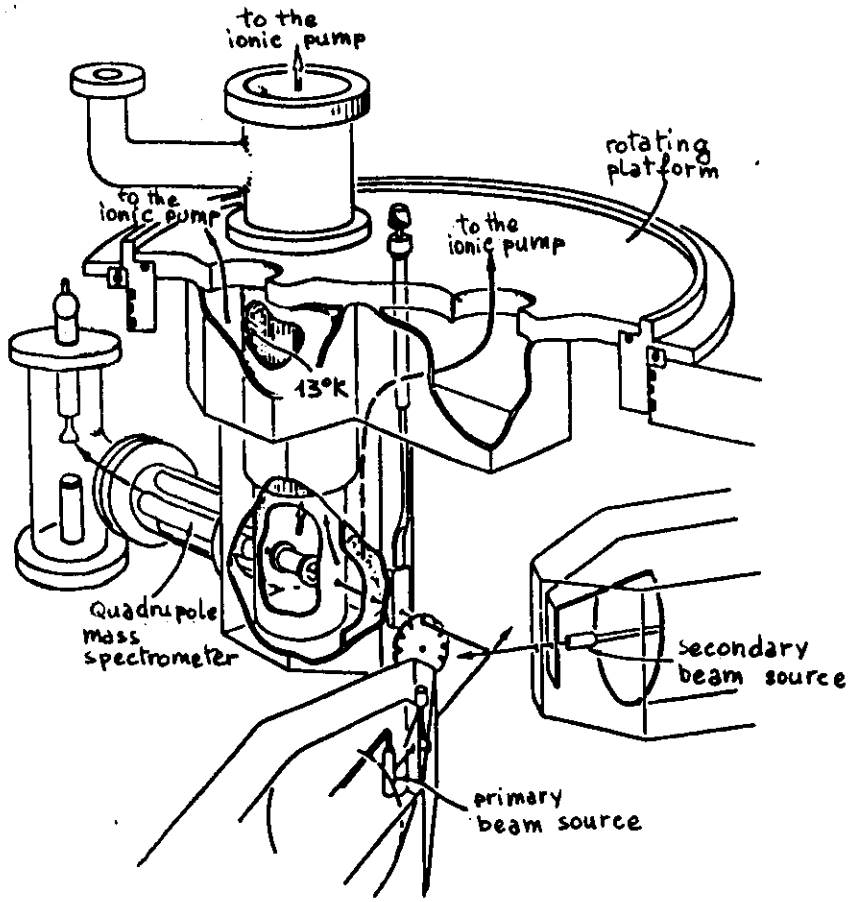


MOLECULAR BEAM APPARATUS FOR INTEGRAL CROSS SECTION

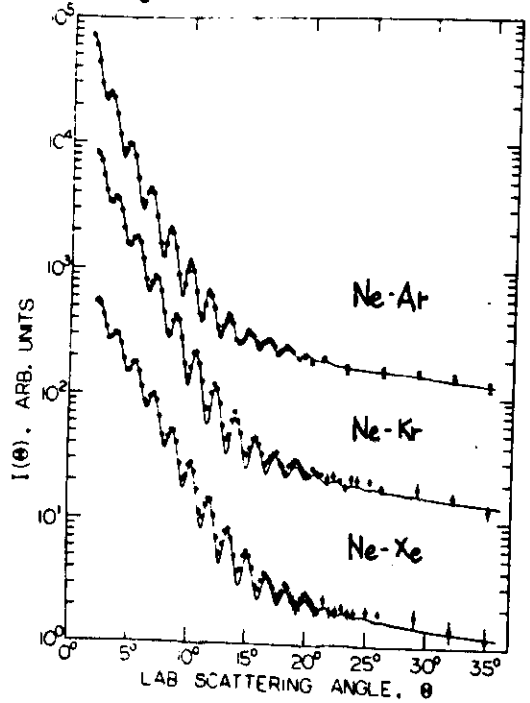




CROSSED BEAM APPARATUS FOR DIFFERENTIAL CROSS SECTION

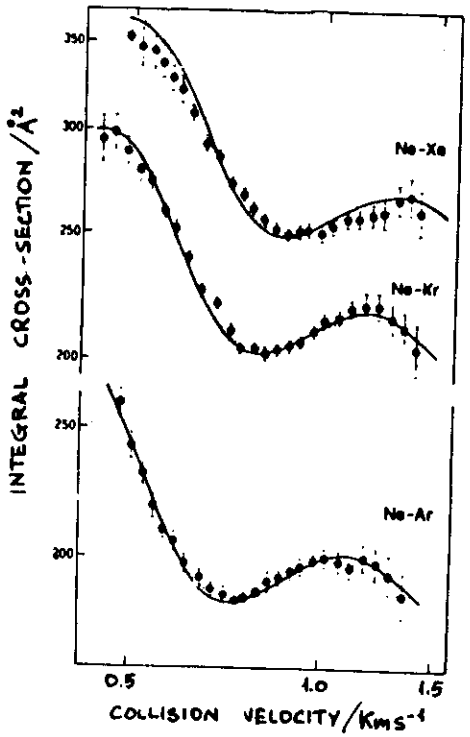


Ne - heavier rare gases



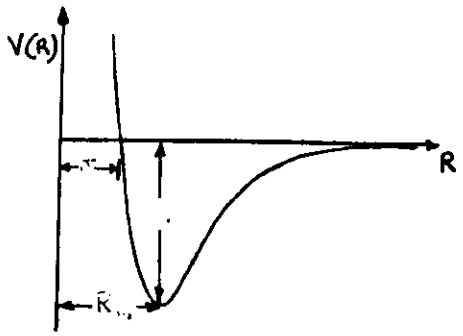
Diffraction structure in the differential cross section (E = 65.4 meV)

Beneventi and Casavecchia (1986)



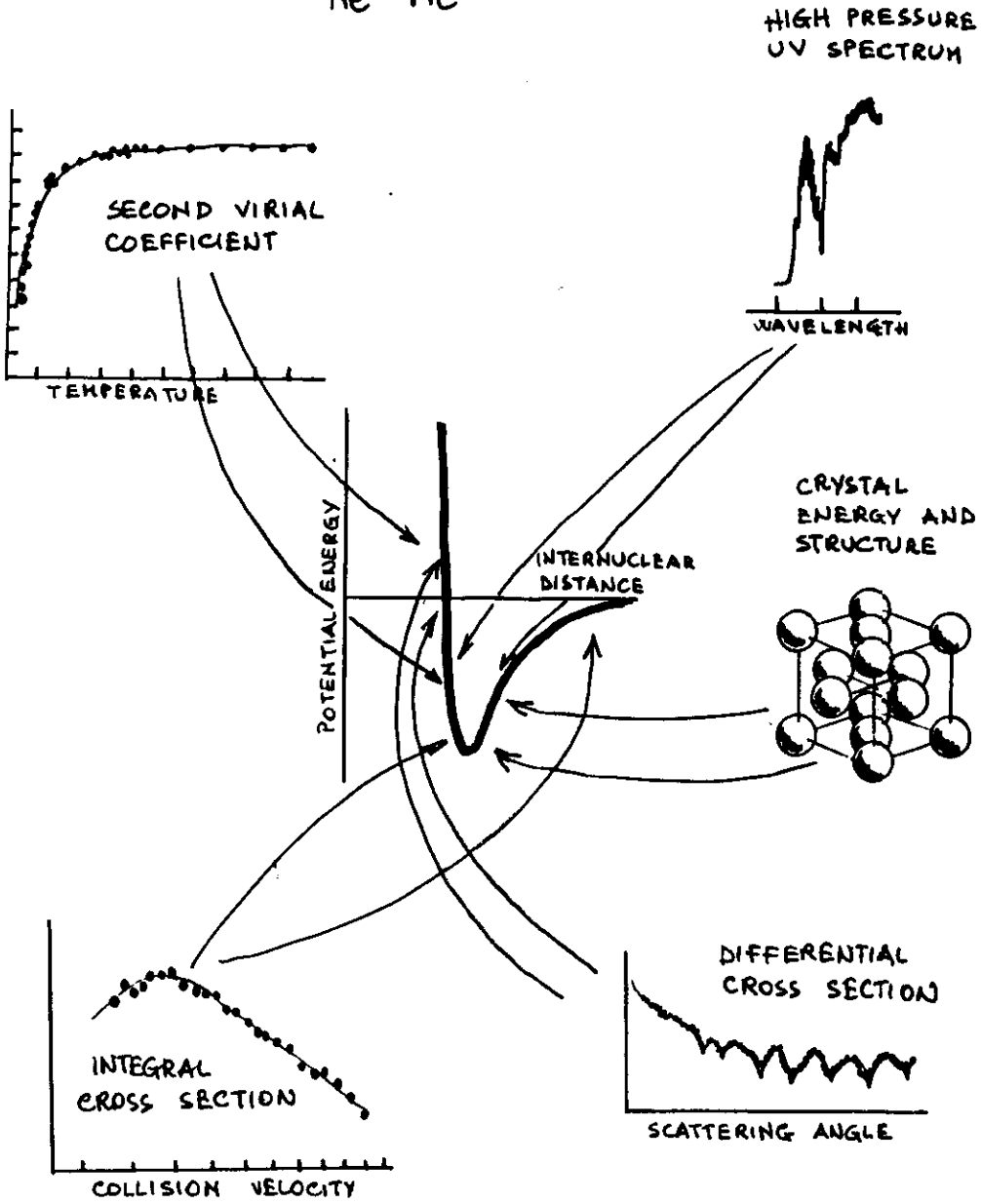
Glory structure in the integral cross section

Candori, Pirani and Vecchiocattivi (1984)



Scattering property	Potential information
Rainbow position	$\sim \varepsilon$
Diffraction undulations	$\sim \sigma$
Glory frequency	$\sim \varepsilon \cdot R_m$
Absolute value of Q(v)	long range attraction

Ne - Ne



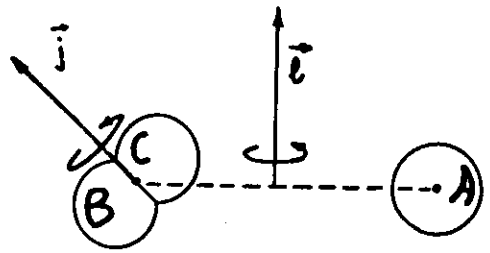
ATOM-ATOM ISOTROPIC INTERACTION

- Scattering properties available today at high level of accuracy (glory, rainbow, diffractio
- Spectroscopic results (vibrational - rotational spacing) available for some systems.
- Equilibrium gaseous properties (virial coefficients) available.
- Dynamical gaseous properties (transport coefficients: diffusion, viscosity, thermal conductivity, etc.) available.

the theory which connects the interatomic potential with the experimental observable is practically exact.

ISOTROPIC INTERATOMIC POTENTIALS ARE KNOWN WITH A HIGH LEVEL OF PRECISION

ATOM - DIATOM INTERACTION (A+BC)



$$\underset{\sim}{U}(R) = \frac{\hbar^2}{2\mu_{BC} r^2}\,\underset{\sim}{j}^2 + \frac{\hbar^2}{2\mu R^2}\,\underset{\sim}{l}^2 + \underset{\sim}{V}(\vec{R})$$

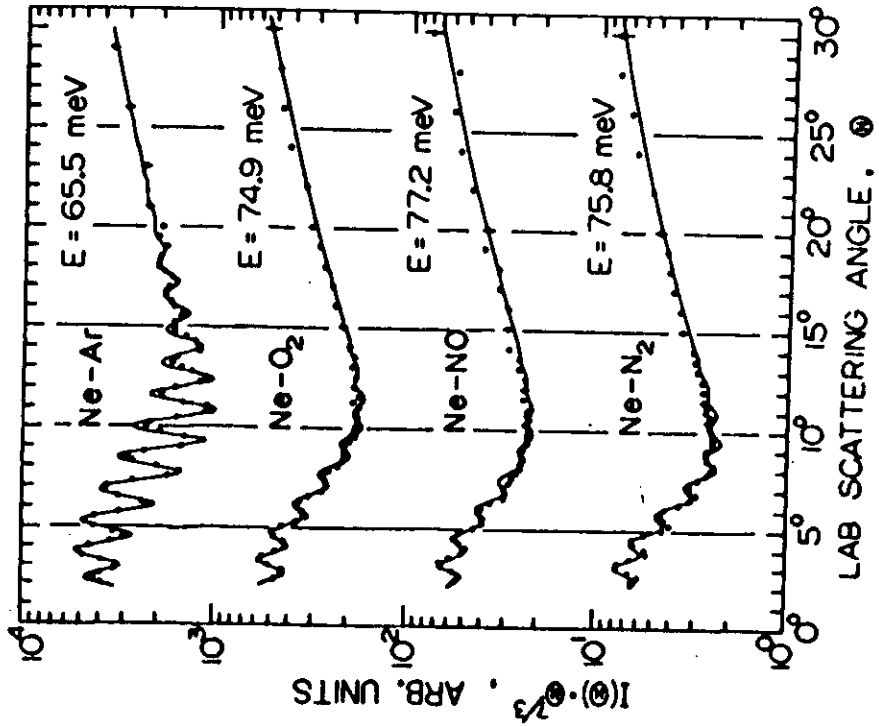
- $\frac{\hbar^2}{2\mu_{BC} r^2}\,\underset{\sim}{j}^2$: rotational term
- $\frac{\hbar^2}{2\mu R^2}\,\underset{\sim}{l}^2$: centrifugal term
- $\underset{\sim}{V}(\vec{R})$: electrostatic term

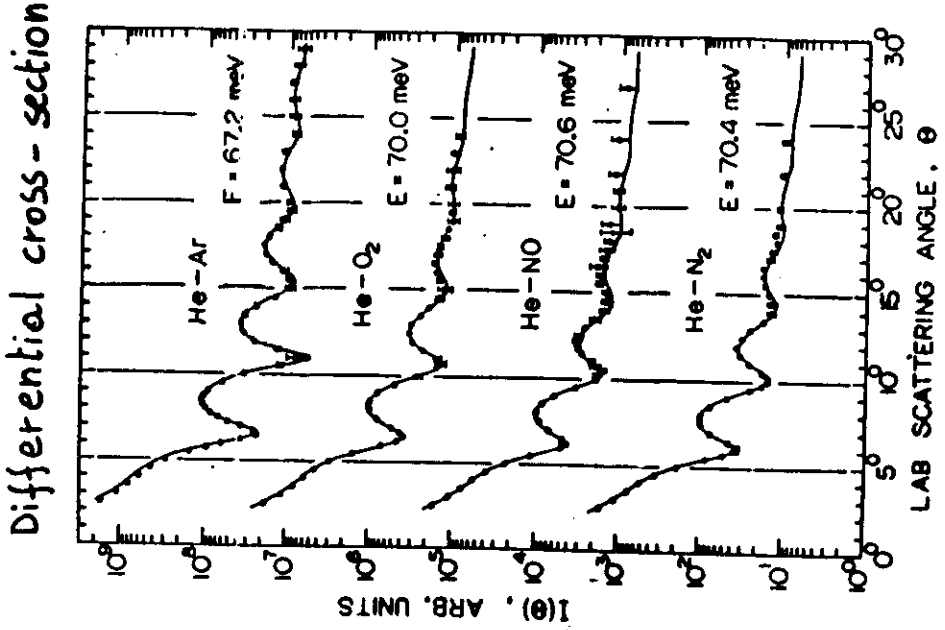
Usual approximations

CENTRIFUGAL SUDDEN (CS) $\quad l(l+1) \simeq \bar{l}(\bar{l}+1)$

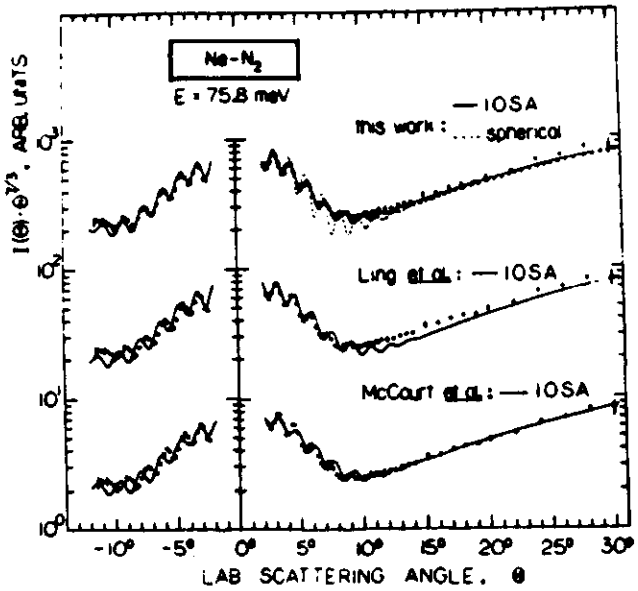
ENERGY SUDDEN (ES) $\quad j(j+1) \simeq \bar{j}(\bar{j}+1)$

INFINITE ORDER SUDDEN (IOS) $\quad IOS = CS + ES$

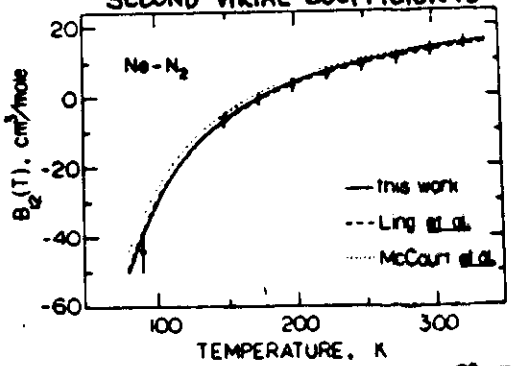




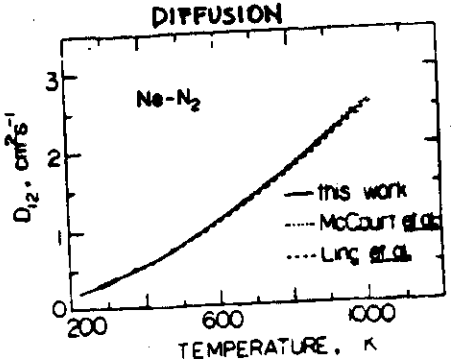
TOTAL DIFFERENTIAL CROSS SECTION

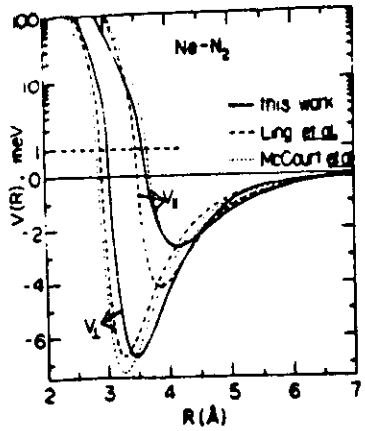


SECOND VIRIAL COEFFICIENTS



DIFFUSION

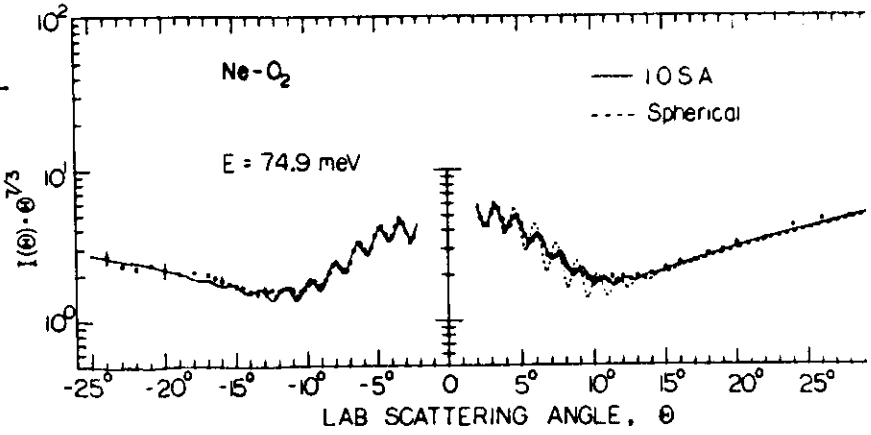




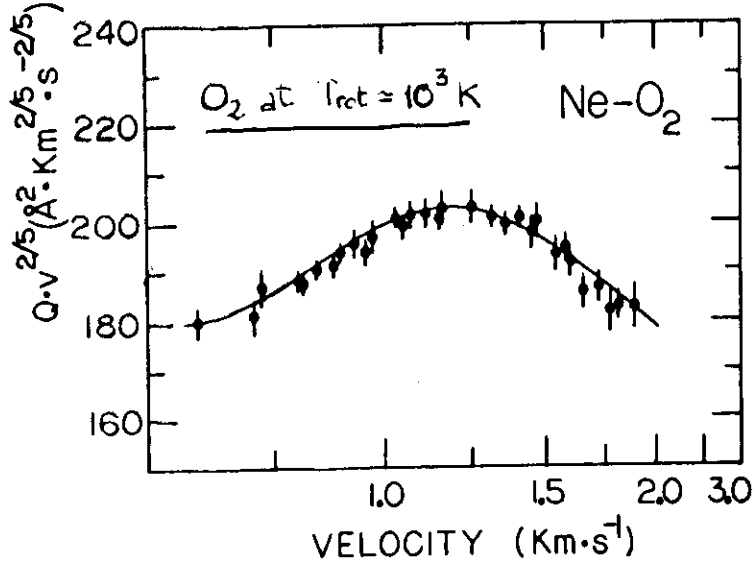
Beneventi, Casavecchia, Pirani, Vecchiocattivi, and Volpi, (1987)

TOTAL DIFFERENTIAL CROSS SECTION

$T_{rot} = 4°K$



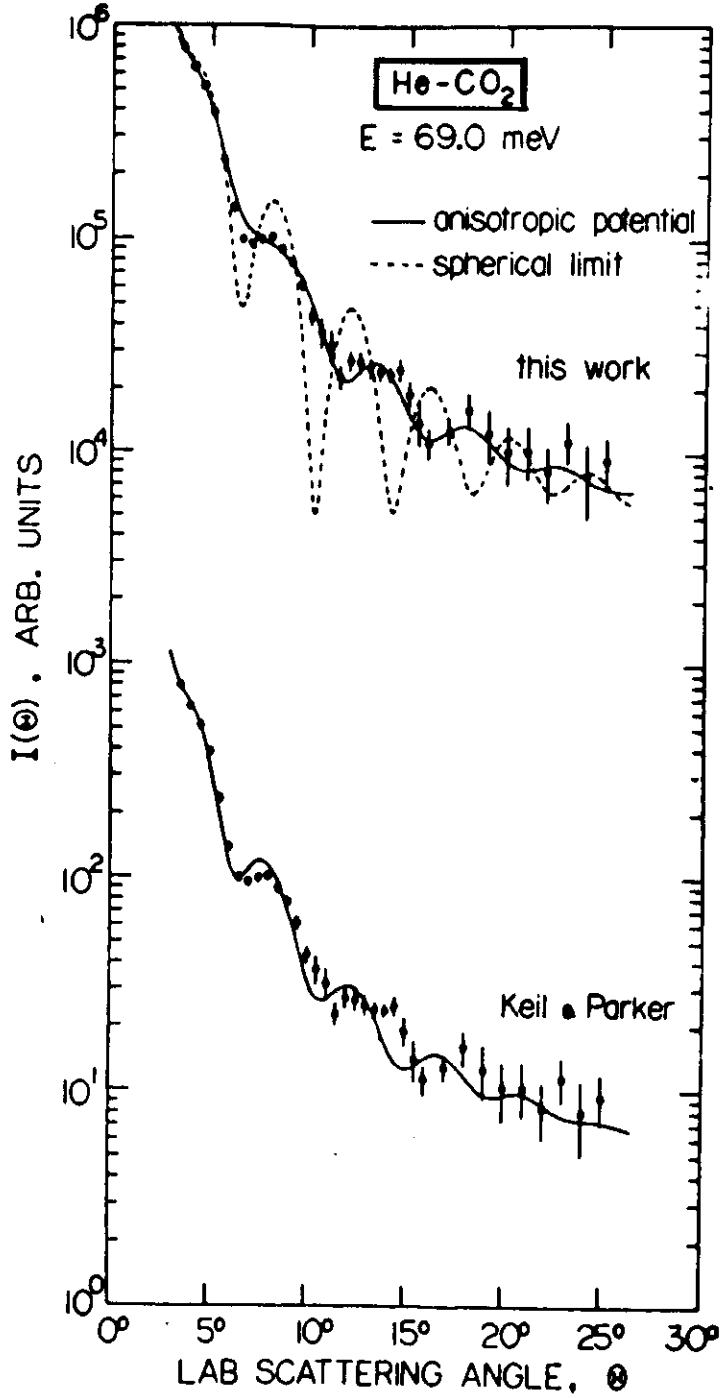
INTEGRAL CROSS SECTION



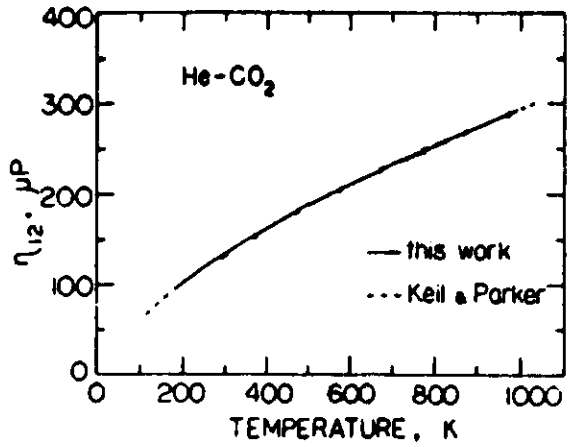
collaboration between Nijmegen & Perugia

T.E.S. ← - total diff. cross section
← - integral cross section
← - spectrum of NeO_2 vdW
← - virial coeff.
transport properties

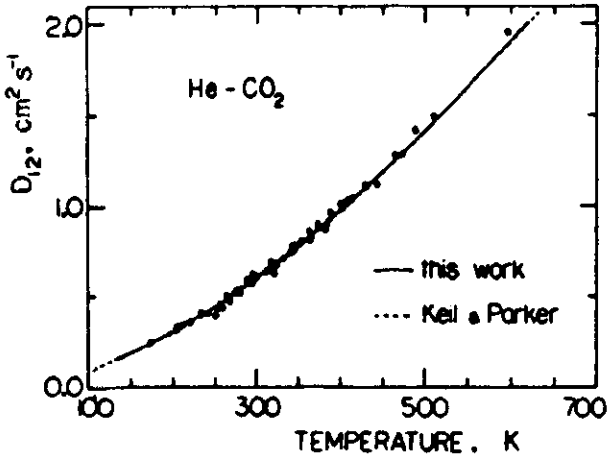
TOTAL DIFFERENTIAL CROSS SECTION



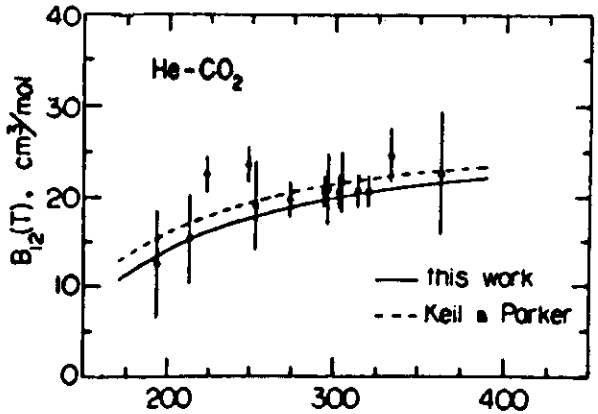
GASEOUS PROPERTIES OF $He-CO_2$ MIXTURE



Viscosity

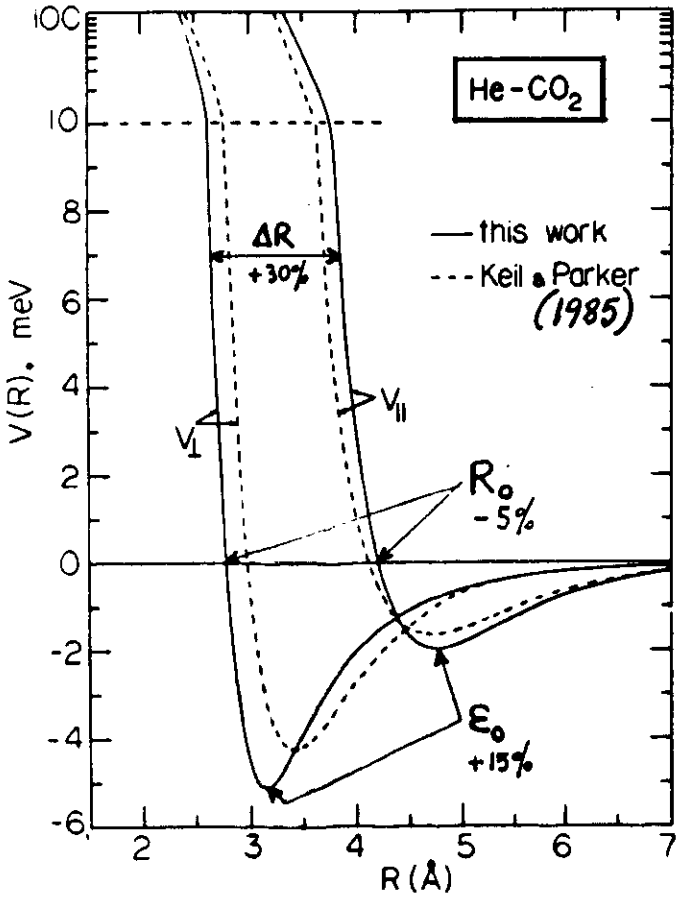


Diffusion



Second virial coefficient

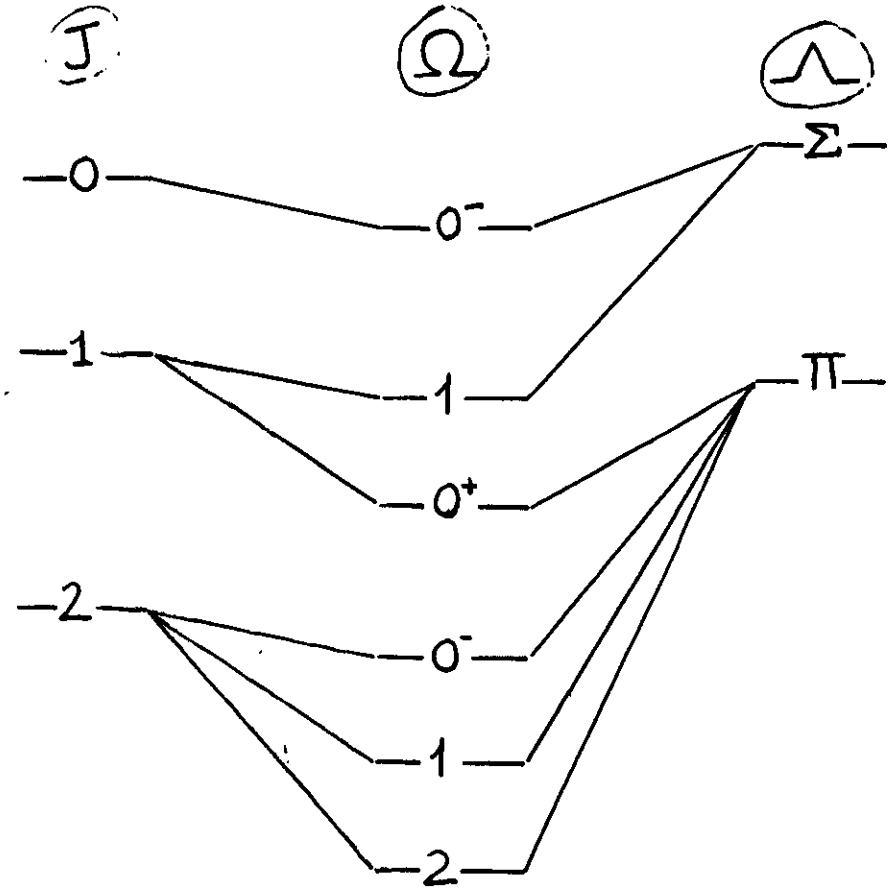
POTENTIAL



L. Beneventi, P. Casavecchia, F. Vecchiocattivi, & G.G. Volpi (PERUGIA)
and
U. Buck, H. Meyer, M. Tolle, & R. Schinke (GÖTTINGEN)

J. Chem. Phys. (1988)

Oxygen - Rare gas $O(^3P_J) - R(^1S_0)$



(e) (c) (a)

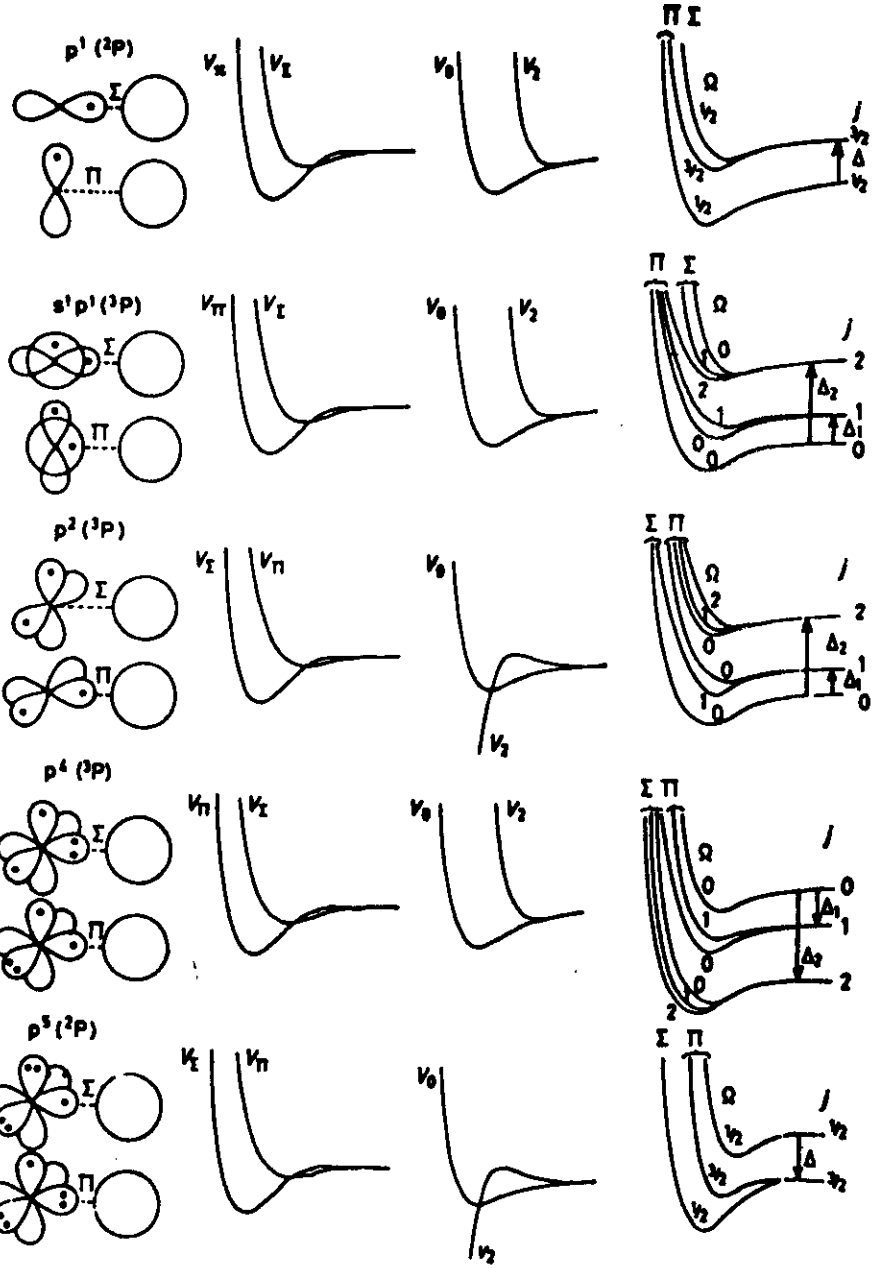
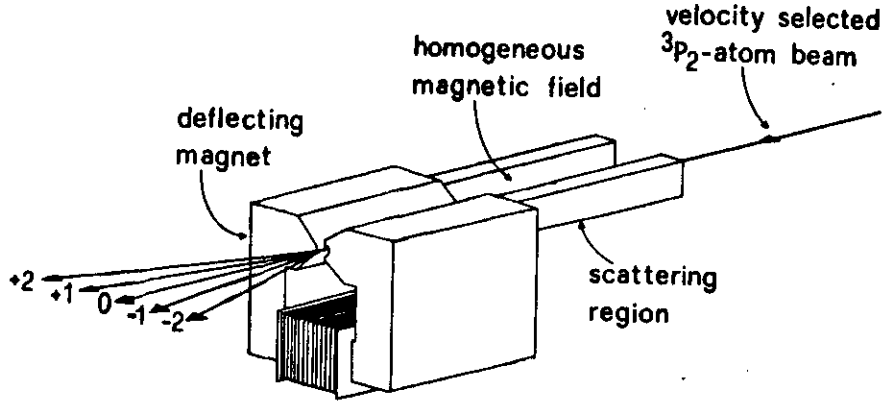


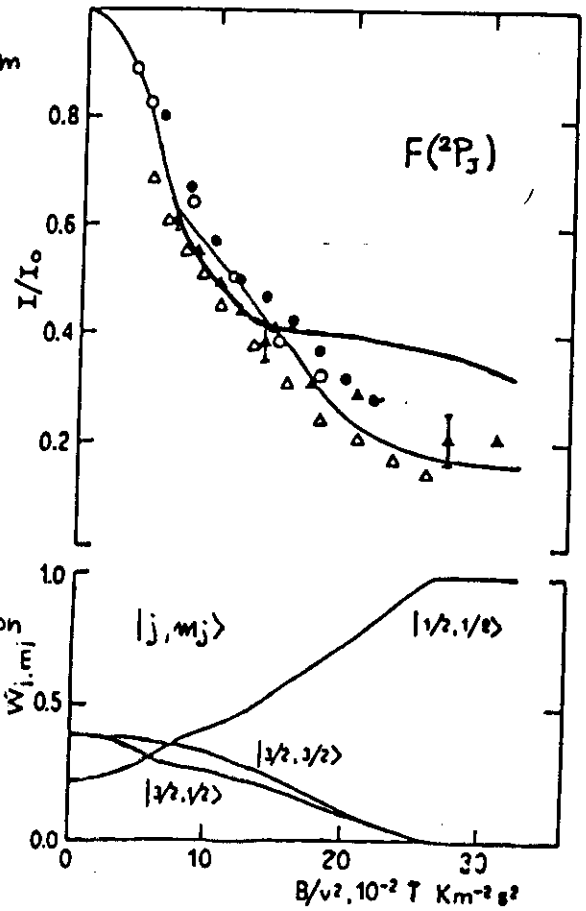
Fig. 2. For typical electronic cloud distributions of open-shell atoms illustrated in the first column, the qualitative behaviour of V_Σ and V_Π interactions with closed-shell systems can be anticipated (second column). The corresponding V_0 (spherical or isotropic interaction) and V_2 (anisotropy) are shown in the third column. The final column shows qualitatively the effective adiabatic interactions, where account is taken of the atomic spin-orbit splitting.



— attenuation assuming no nuclear spin decoupling for $j=3/2$

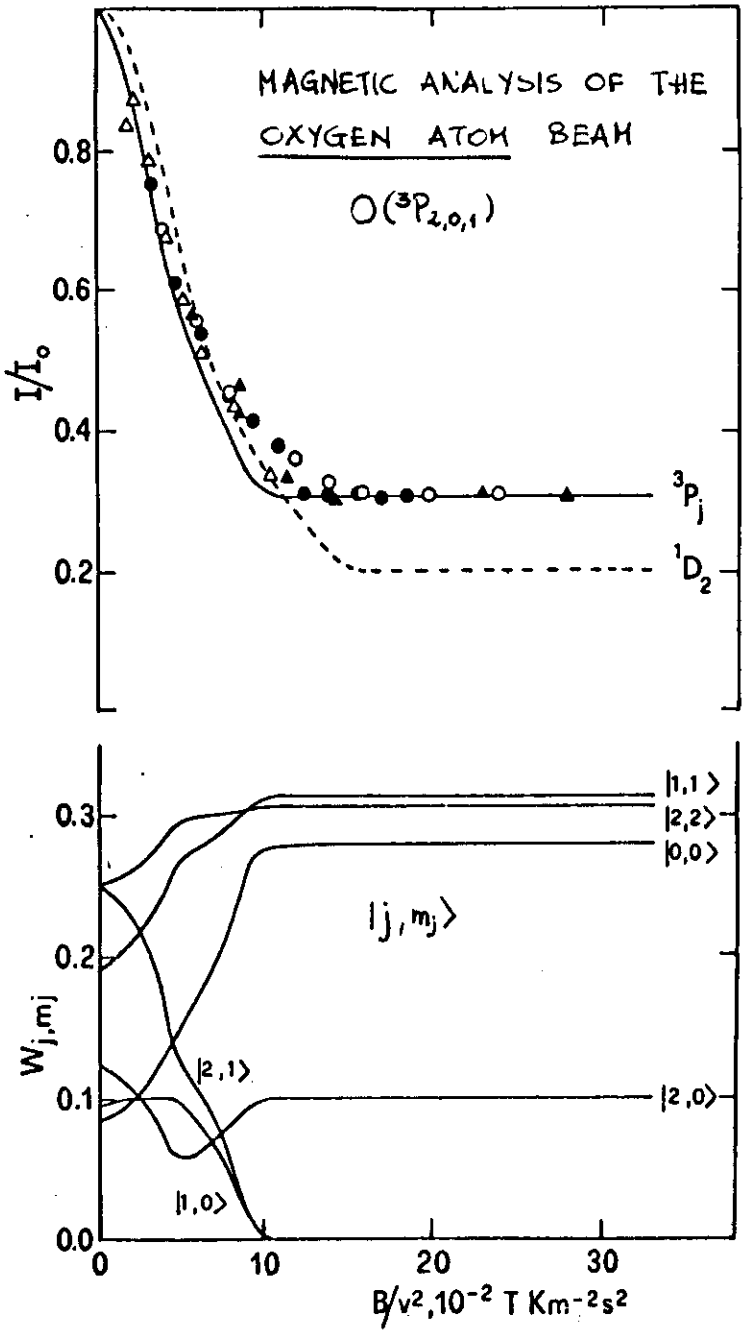
— attenuation assuming decoupling

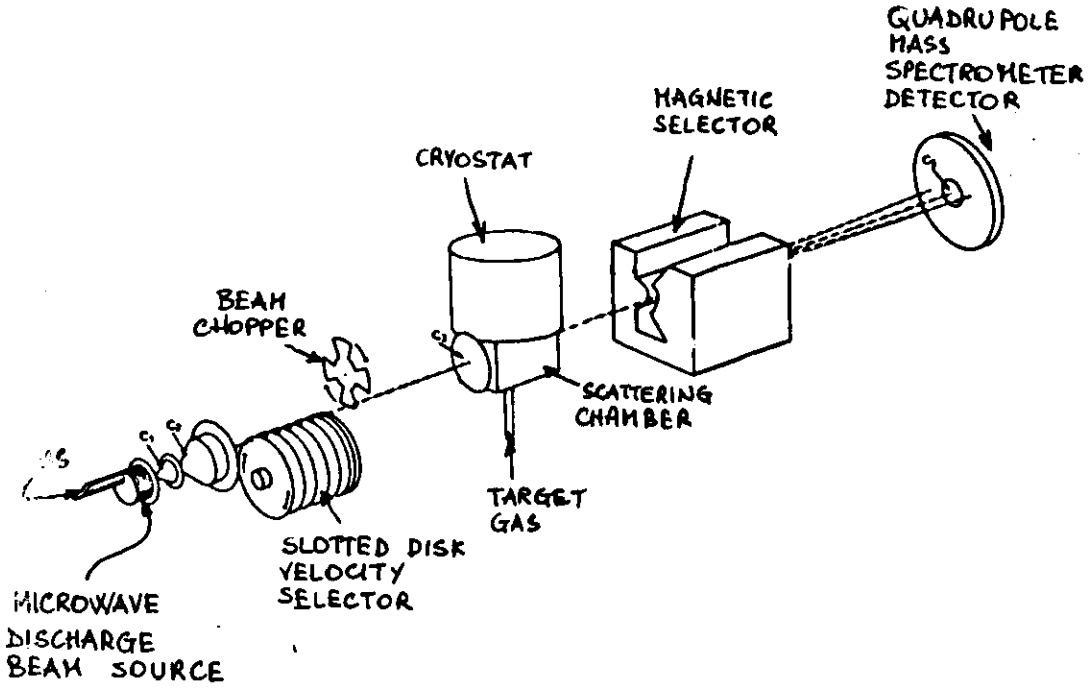
Fluorine atom beam attenuation as a function of B/v^2



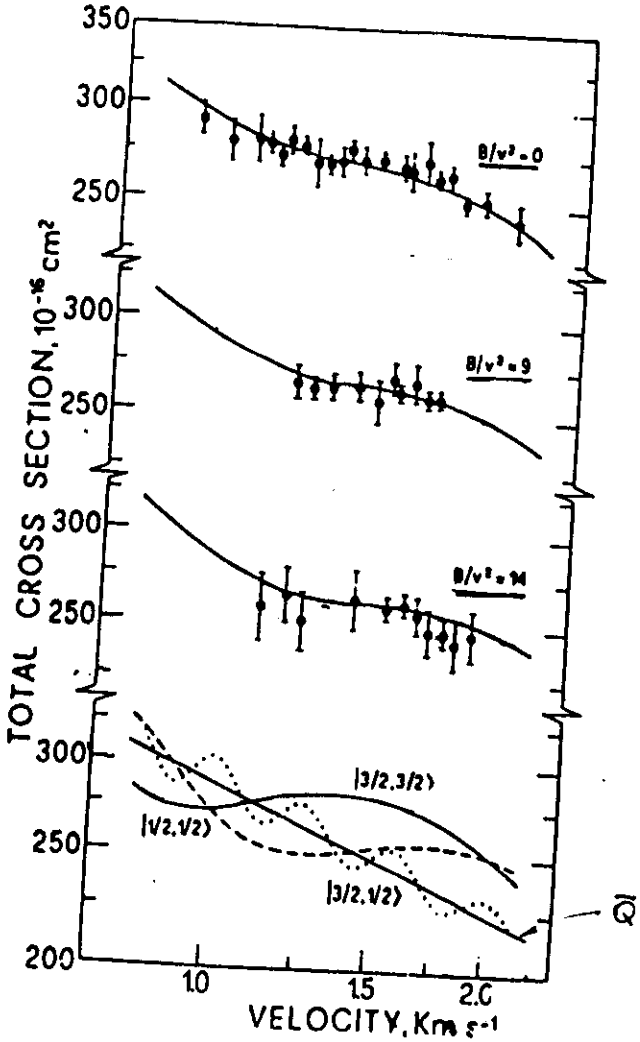
$|j,m_j\rangle$ concentration

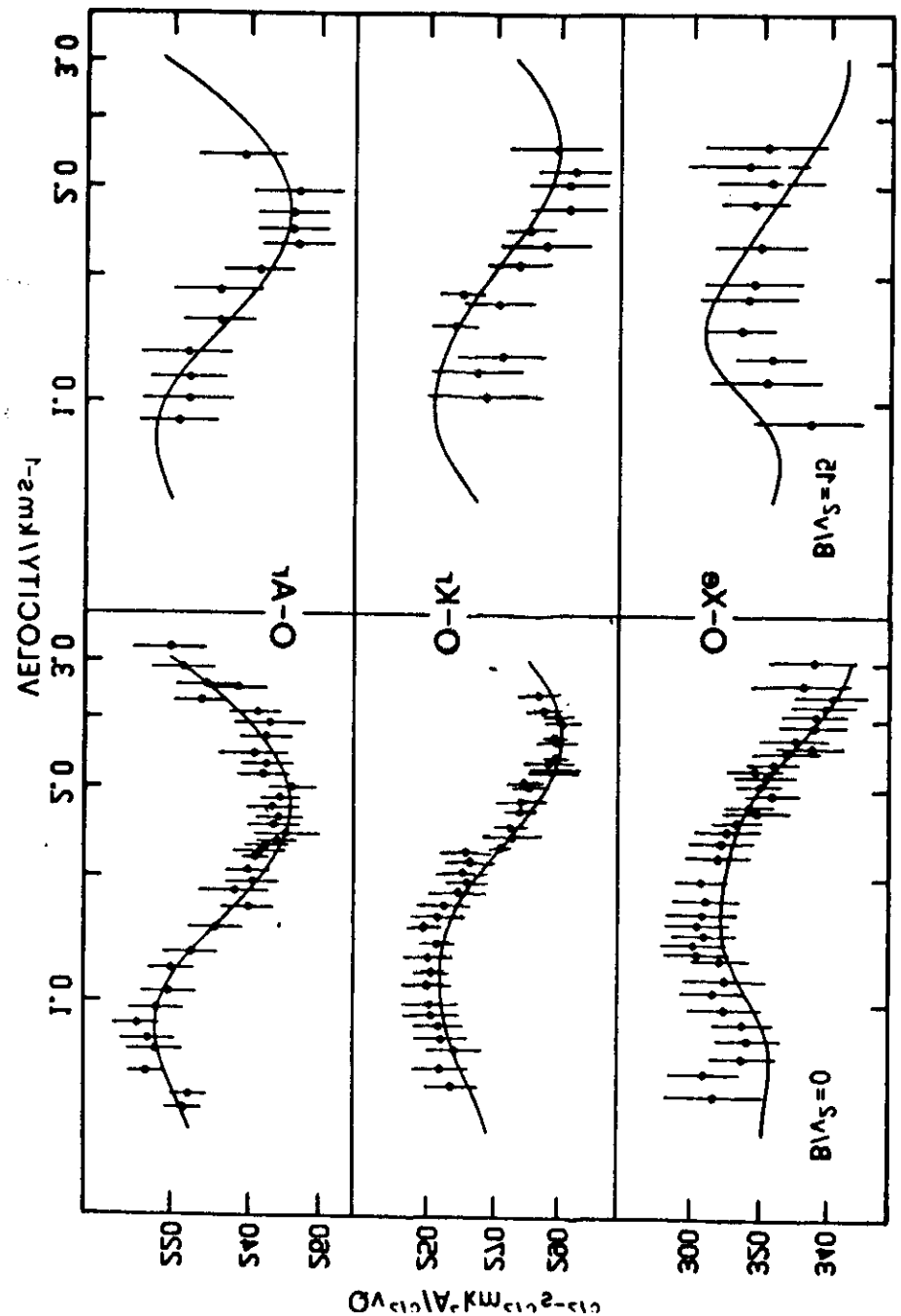
Beam attenuation as a function of B/v^2



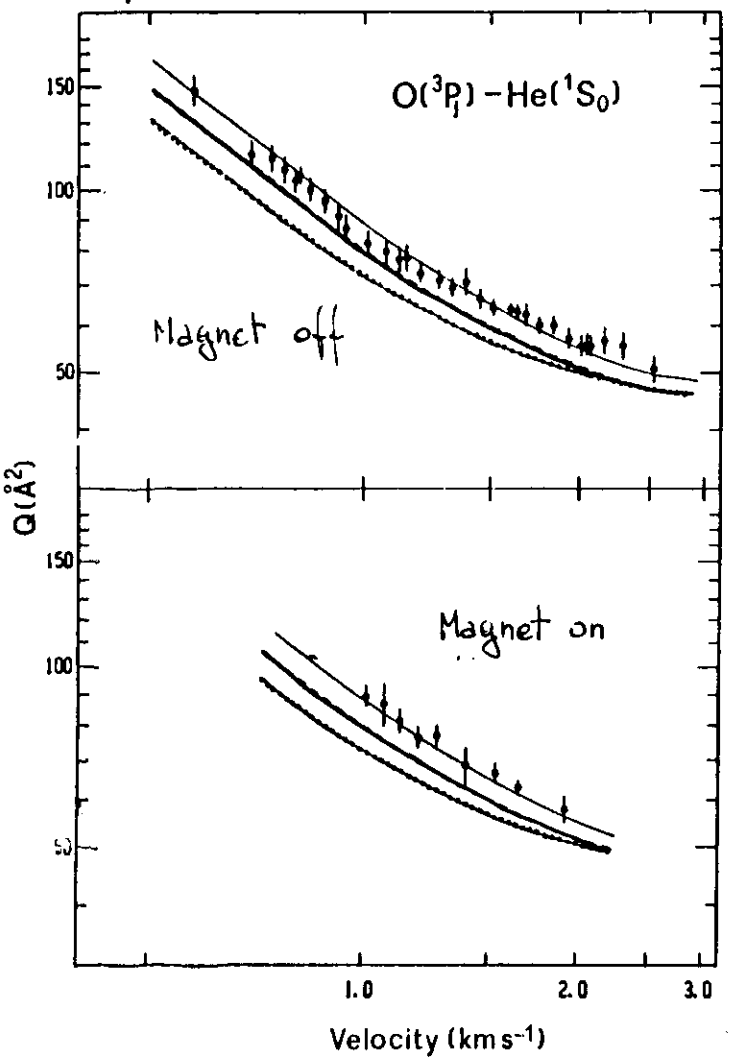


$F(^2P_{1/2,3/2}) + Xe(^1S_0)$

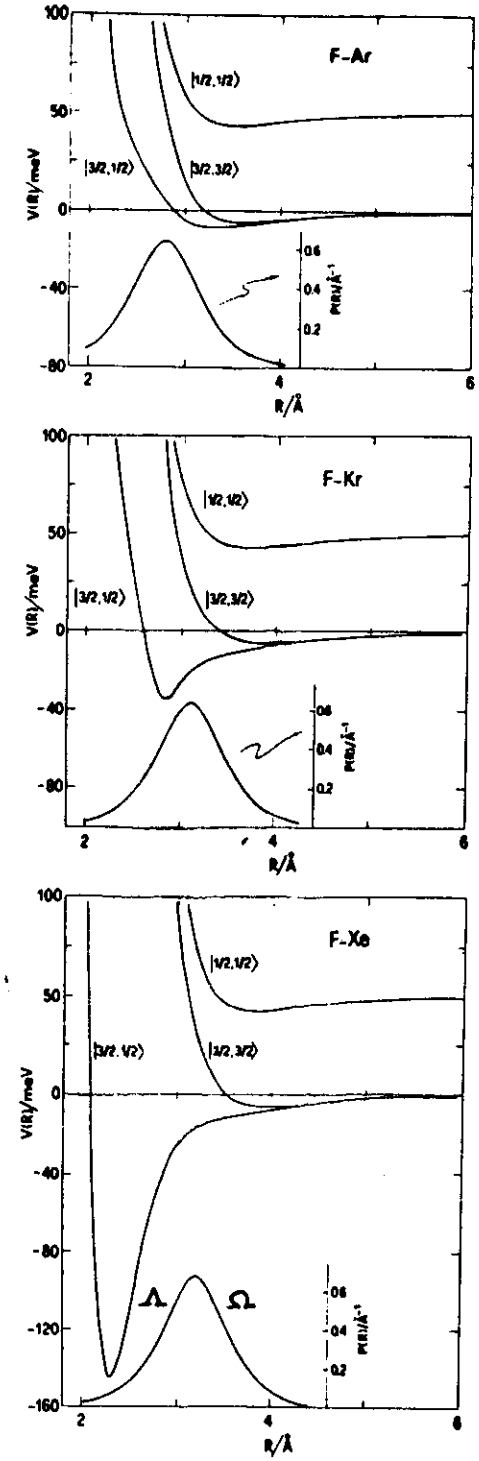




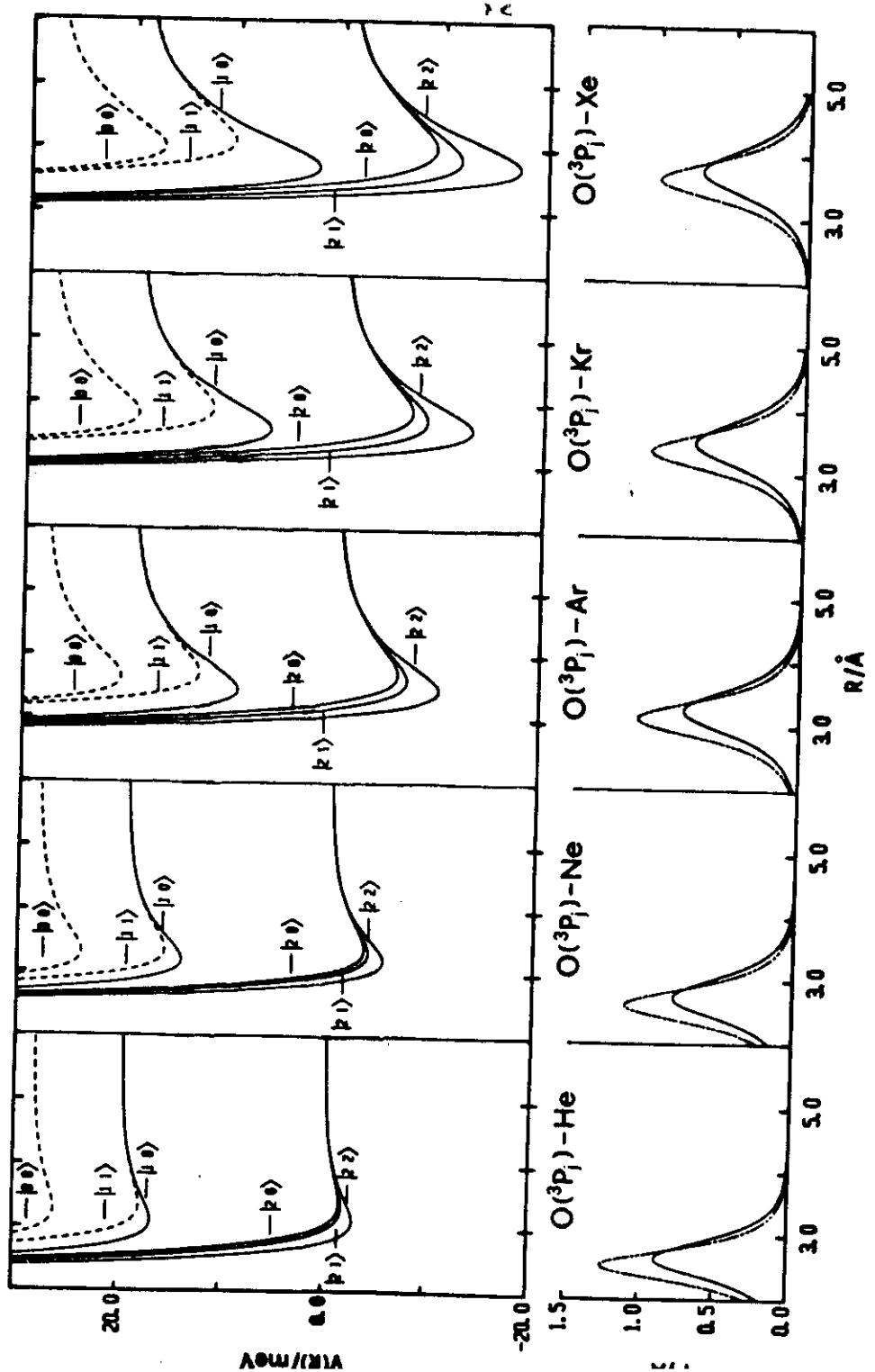
Aquilanti et al., J.C.P. (1986)



— CEPA calculations by Staemmler and Jaquet (19
— extrapolated results by Staemmler and Jaquet (1985)

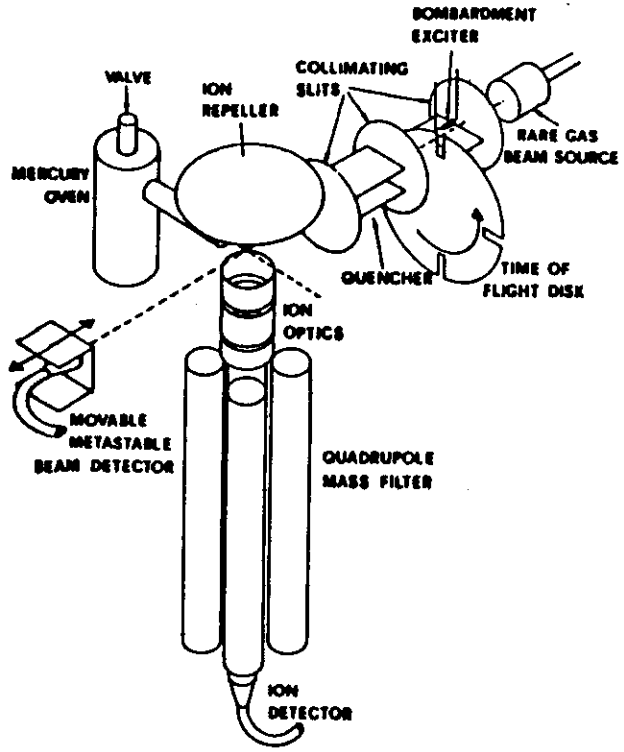


Amilanti Pirani and Vecchiocattivi (1987)



Metastable rare-gas atoms

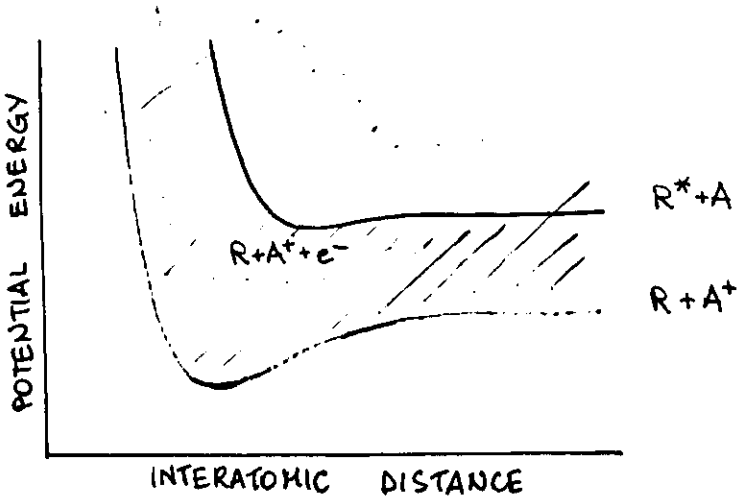
$He^*(2^3S, 2^1S)$
$Ne^*(^3P_{2,0})$
$Ar^*(^3P_{2,0})$
$Kr^*(^3P_{2,0})$
$Xe^*(^3P_{2,0})$

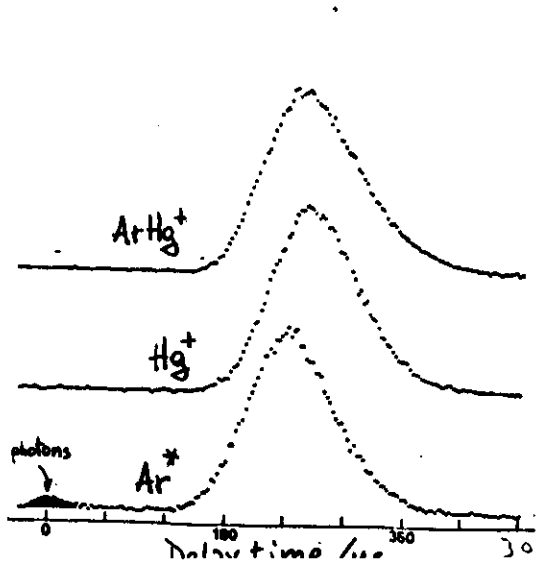


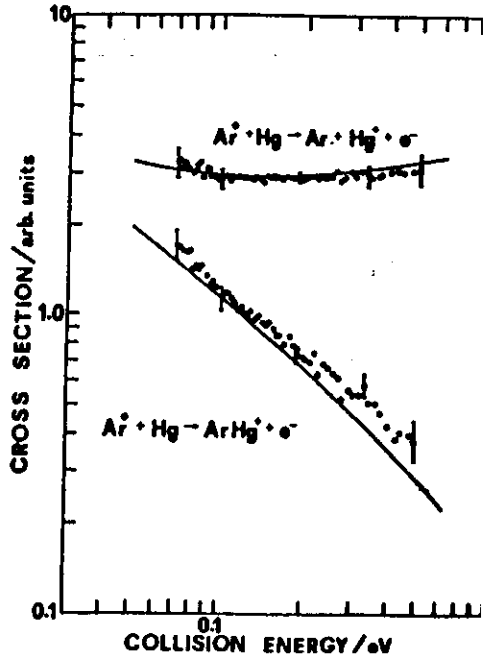
$$R^* + A \longrightarrow R + A^+ + e^- \quad \text{Penning ion.}$$
$$\longrightarrow RA^+ + e^- \quad \text{associative ion.}$$

Electronic energy of R^* > Ionization potential of A

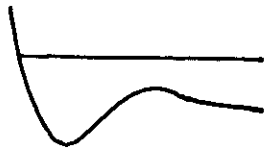
$$Ar^*(^3P_{2,0}) + Hg \rightarrow Ar + Hg^+ + e^-$$
$$\rightarrow ArHg^+ + e^-$$







$$R^* + A \rightarrow (RA^+) + e^-$$



$R + A^+$
Penning ionization

RA^+
Associative ionization

$(RA^+) \xrightarrow{\tau} R + A^+$
Quasi-associative ionization