Low Energy Electron Scattering Cross Sections: Measurements and Calculations

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Outline

- The need for electron cross section information ?
- Cross Section Definitions
- Where are we experimentally ?
  - what can we measure and how accurately
- Experimental Techniques
- Theoretical Approaches
- Atomic structure
- Some typical examples of cross sections
- Resonance Scattering
- Excited States
- Radicals

NOTE : A few new slides and additions !)

Electron Scattering

Interesting from fundamental perspective

Electron scattering is relevant to many areas of applied science

- astronomy and astrophysics
- gas discharge physics and devices
  - laser and lighting science
  - surface modification of materials
- fusion science plasmas
  - materials research
- biomedical science
- environmental science
- ..... etc

Important Processes

- Elastic Scattering – no energy exchange

$$e^- + AB \rightarrow e^- + AB$$

- Inelastic Scattering – many possibilities

$e^- + AB \rightarrow e'^- + (AB)^*$ inelastic electron

Vibration, rotation, electronic excitation

$\rightarrow AB + h\nu$ photon emission

$\rightarrow (AB)^*$ metastable atom/molecule

- Breakup Reactions

$e^- + AB \rightarrow e' + (AB)^+$ Ionization

$e^- + AB \rightarrow e' + A + B$ Dissociation

$e^- + AB \rightarrow A + B^-$ Dissociative Attachment

- Excited States

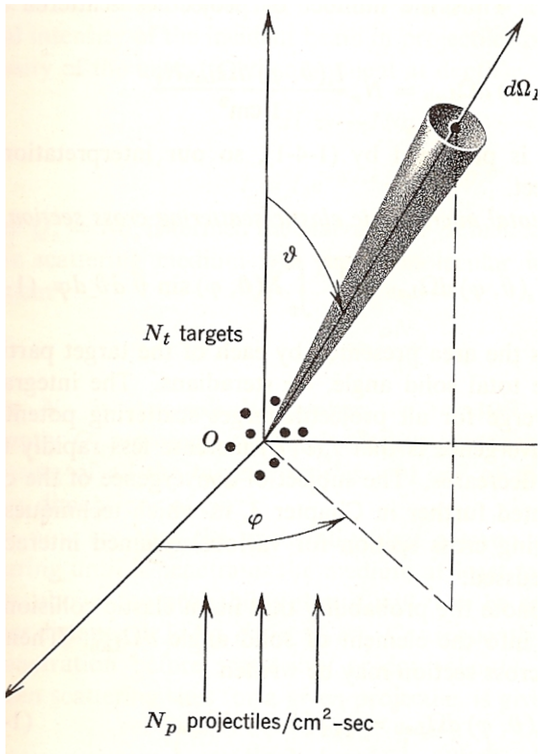
$e^- + (AB)^* \rightarrow$ all of the above are possible + !

What is a cross section?

- A measure of the scattering probability
  - The results (or magnitude) of a collision are usually expressed in terms of a collision cross section (or sometimes a Rate Coefficient). The cross section is defined as the ratio of the number of collisions per unit time, per unit scatterer, to the flux of incident projectile particles. It can be considered as a measure of the probability of a particular type of collision occurring under a given set of conditions.
  - for electron collisions cross sections are generally expressed as a function of energy (E) OR scattering angle (θ) OR both E and θ
  - cross sections have the dimension of area (or area per element of solid angle) – $Å^2$, a_0^2, πa_o^2, ...
  - "typical" electron scattering cross section – 10^{-16} cm^2 or 1 $Å^2$

Types of Cross Section

- TOTAL Cross Section
  - This cross section represents the total 'area' that each target particle presents to the projectiles for scattering into all space – i.e. the full 4π steradians of solid angle. The total cross section is usually referred to as Q_T or σ_T
- DIFFERENTIAL Cross Section
  - Often referred to as $d\sigma/d\Omega$ the differential cross section per unit solid angle.
  - $d\sigma$ can be considered classically as the 'area' presented by the target particle to the projectiles for scattering into the element of solid angle $d\Omega$



Types of Cross Section

- INTEGRAL Cross Section
  - The integral cross section for a particular process, e.g. elastic scattering – usually referred to as Q_i or σ_i – is obtained by integration of the differential cross section over all scattering angles (sometimes confused with total scattering cross section)

$$\sigma_i = \int \frac{d\sigma}{d\Omega} d\Omega$$

$$= \int_0^{\pi} \int_0^{2\pi} \frac{d\sigma}{d\Omega} \sin\theta \, d\theta \, d\phi$$

$$= 2\pi \int_0^{\pi} \frac{d\sigma}{d\Omega} \sin\theta \, d\theta$$

Types of Cross Section

- MOMENTUM TRANSFER Cross Section
  - a cross section often used to characterise scattering in low temperature plasmas/discharges
  - an effective cross section that represents the average momentum transfer between projectile and target
  - weighted for "backward scattering"

$$\sigma_m = \int (1-\cos\theta)\frac{d\sigma}{d\Omega}d\Omega$$

$$= \int_0^{\pi}\int_0^{2\pi} \frac{d\sigma}{d\Omega}(1-\cos\theta)\sin\theta\, d\theta\, d\phi$$

$$= 2\pi\int_0^{\pi} \frac{d\sigma}{d\Omega}(1-\cos\theta)\sin\theta\, d\theta$$

Other Popular Parameters

- MEAN FREE PATH
  - The AVERAGE distance between scattering events

$$\lambda = \frac{1}{NQ_T}$$

N= number density

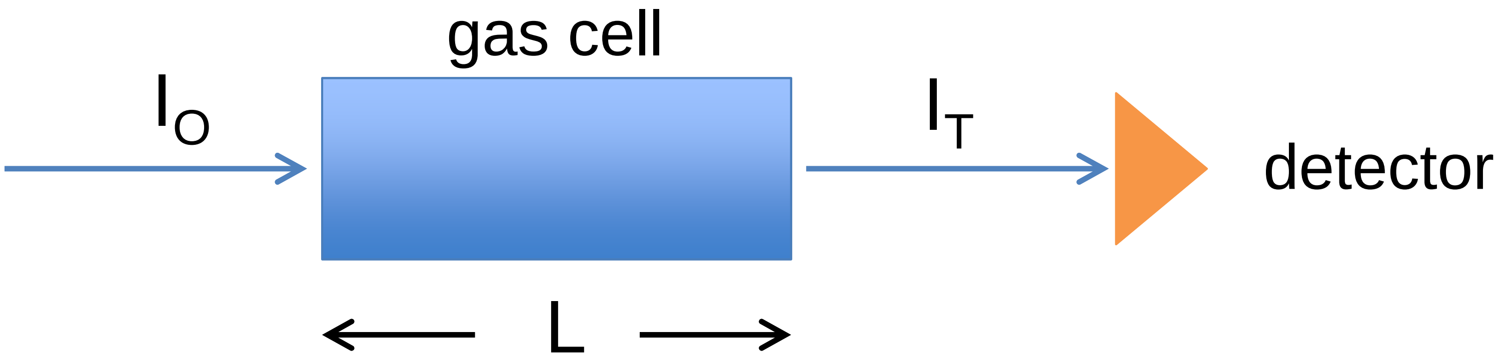
- RATE COEFFICIENTS
  - In many cases collision probabilities for *inelastic* scattering are described in terms of a rate coefficient rather than a cross section
  - The rate coefficient is the integrated product of the Cross section, the energy and normalised energy distribution

$$k = \int_0^\infty EQ(E)\, f(E)\, dE$$

($cm^3 s^{-1}$)

BEER-LAMBERT LAW

- A generic expression for the absorption of particles
  - used in radiation, scattering, ...
- TOTAL CROSS SECTION
  - consider I_o particles incident on a gas cell of number density N



$$Q_T = \ln\left(\frac{I_0}{I_T}\right)\frac{1}{NL}$$

Other Relationships

- Scattering Channels
  - At a given energy a number of processes may be energetically possible – these are called “open scattering channels”
  - For all open channels, *i*

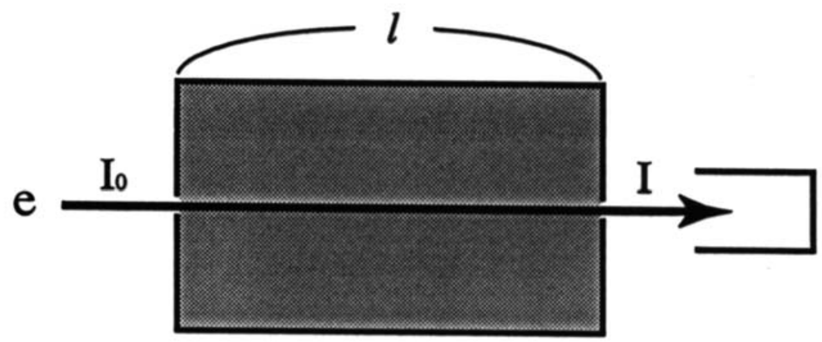
$$Q_T = \sum_i Q_i$$

  - The total cross section is the limiting parameter for all processes – open channels - at a given energy

Experimental measurements

- What do we want to measure ?
  - absolute cross sections
  - energy dependence
  - angular dependence
  - energy sharing in breakup
- What do we need ?
  - beam of atoms/molecules or gas cell
    - characterised for number density (pressure, temperature)
  - beam of electrons
    - preferably monochromatic (high resolution - resolve vibration/rotations)
  - Energy analysis of scattered particles
  - Detectors (electrons, photons, excited atoms)

Experimental Techniques



Transmission experiment

- measures total scattering

detect UNSCATTERED particles

- so NOT a scattering experiment

$$I = I_0 e^{-Q_T N l}$$

$$Q_T = \sum_n q_n$$

※Upper limit of cross sections

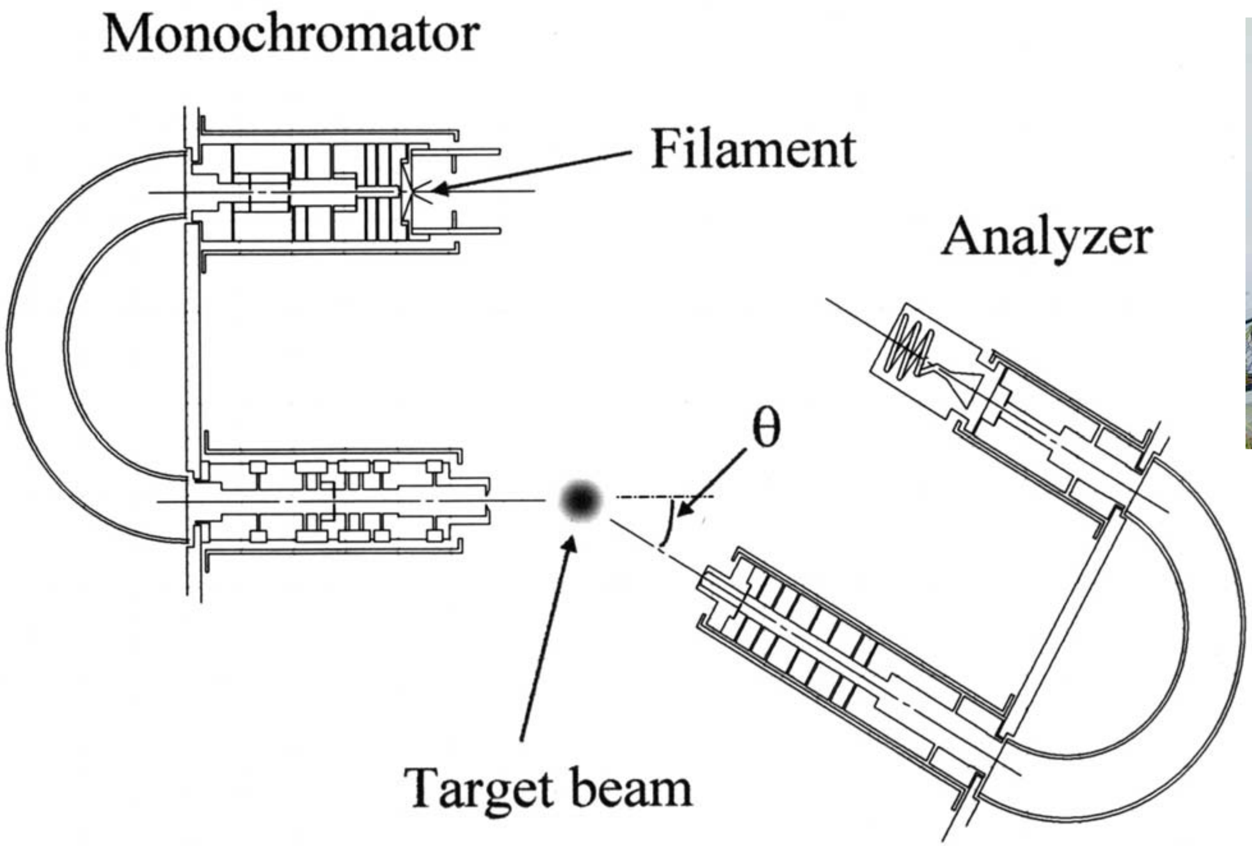
Single collision conditions

Courtesy of H. Tanaka

Experimental Techniques

Crossed beam method – angular differential cross sections

Single collision conditions & high energy resolution (~20 meV)

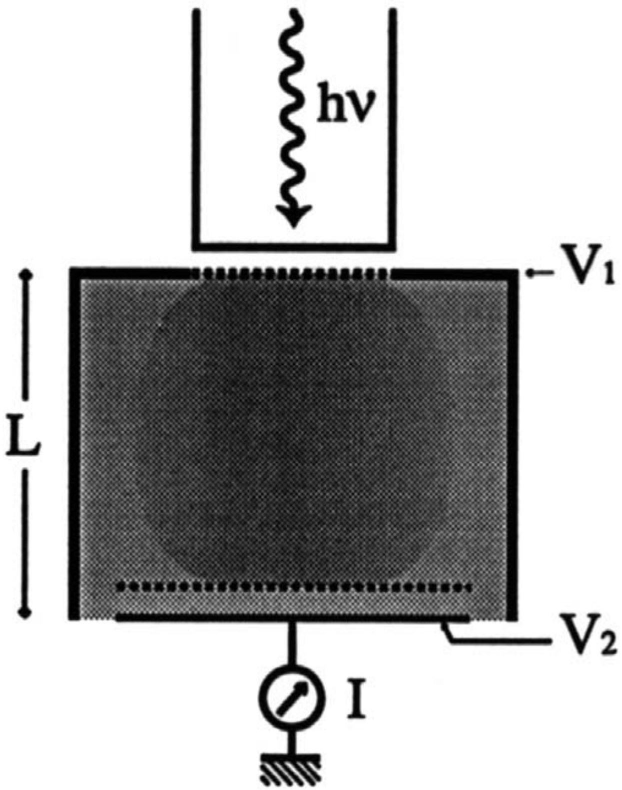


Typical crossed-beam electron spectrometer

Courtesy of H. Tanaka

Swarm experiment – high pressure gas, multiple collisions,

measure transport parameters – drift, diffusion



Courtesy of H. Tanaka

Boltzmann equation

$$\partial f/\partial t + v \cdot \nabla_X f + (F/m) \cdot \nabla_v f = [\partial f/\partial t]_c$$

Measurables - electrons

What can we measure ?

- Accurately
  - Total scattering
    - typically ±3-5%
  - Elastic Scattering
    - differential ~10%
    - integral ~25%
  - Vibrational Excitation
    - differential ~15-20%
    - integral ~25-30%
  - Ionization
    - typically 3-5% (total)

- Not so Accurately
  - Electronic Excitation (~30%)
  - Dissociative Attachment
  - excited state collisions
  - collisions with radicals

- "Almost impossible"
  - neutral dissociation

Theory

- Experiment can only accurately measure ~10% of what is required !
- Must use theoretical estimates
- High Energies – many approaches
  - Born Approximation, semiclassical, perturbative
- Low Energies – very complicated (but interesting !)
  - full quantum scattering theory required
  - solution of Schrödinger equation (Dirac Equation)

$$H\Psi = E\Psi$$

H – Hamiltonian, KE, Coulomb, Exchange, Polarization, ...

Ψ - Total wave function, electron + target

Theory – cont'd

$$H = -\frac{1}{2}\nabla^2 + V_s(r) - V_{ex}(r) + V_{pol}(r) + V_{so}(r) + V_{dip}(r) + \ldots\ldots$$

Static Coulomb Interaction $$V_s(r) = -\frac{Z}{r} + \sum_{j=1}^{Z} \frac{1}{\left|r - r_j\right|}$$

Exchange Interaction $$V_{ex}(r) \propto AN(r)^{1/3} F$$

Polarization potential $$V_p(r) \approx -\frac{\alpha}{2r^4}$$

Spin-Orbit Interaction $$V_{SO}(r) \propto \frac{Z}{r}\frac{dV}{dr}\,\underline{s} \bullet \underline{l}$$

Dipole Potential $$V_D(r) \approx -\frac{eD}{r^2}\cos\chi$$

Theory

- Most processes can be calculated – but how well ?
  - for atomic systems - theory in excellent shape
    - CCC method, R-matrix method, Variational methods
  - for small molecules – also highly reliable for some processes
    - R-matrix, Kohn Variational, Schwinger Variational, ...
  - For large molecules, many problems
    - some success
- Must benchmark theory and experiment
  - theory needs to be major provider
  - benchmark using processes where experiment is accurate
    - total scattering, differential elastic, ionization, ...
    - atoms & simple molecules

Cross Sections – some examples

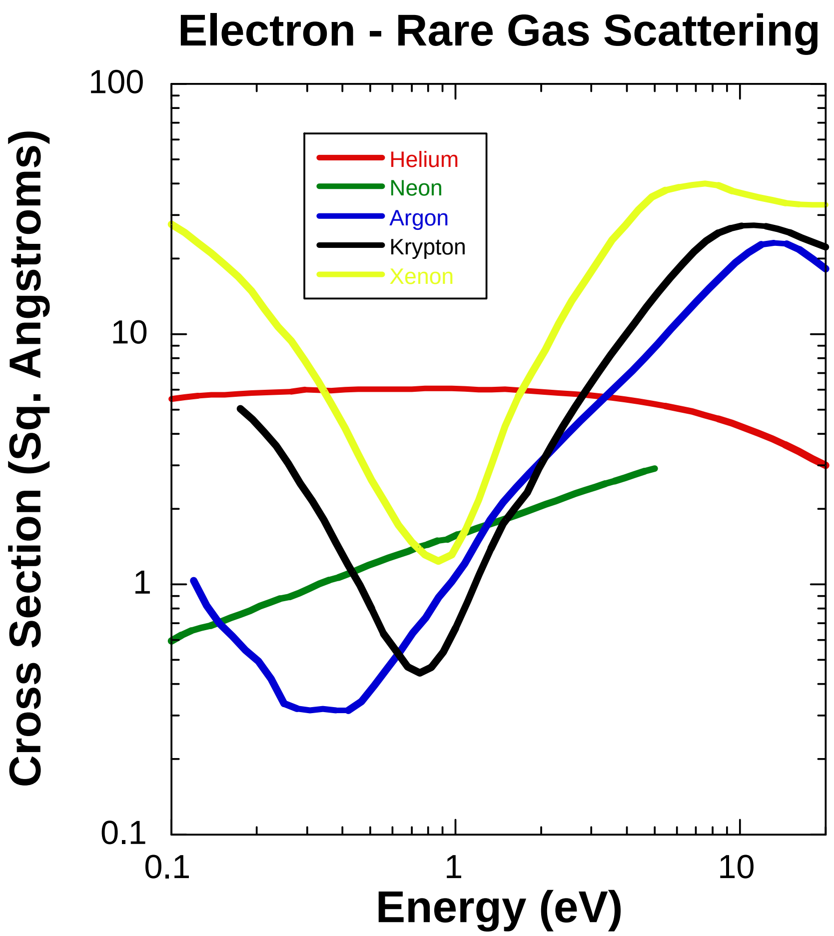
TOTAL SCATTERING

RARE GASES

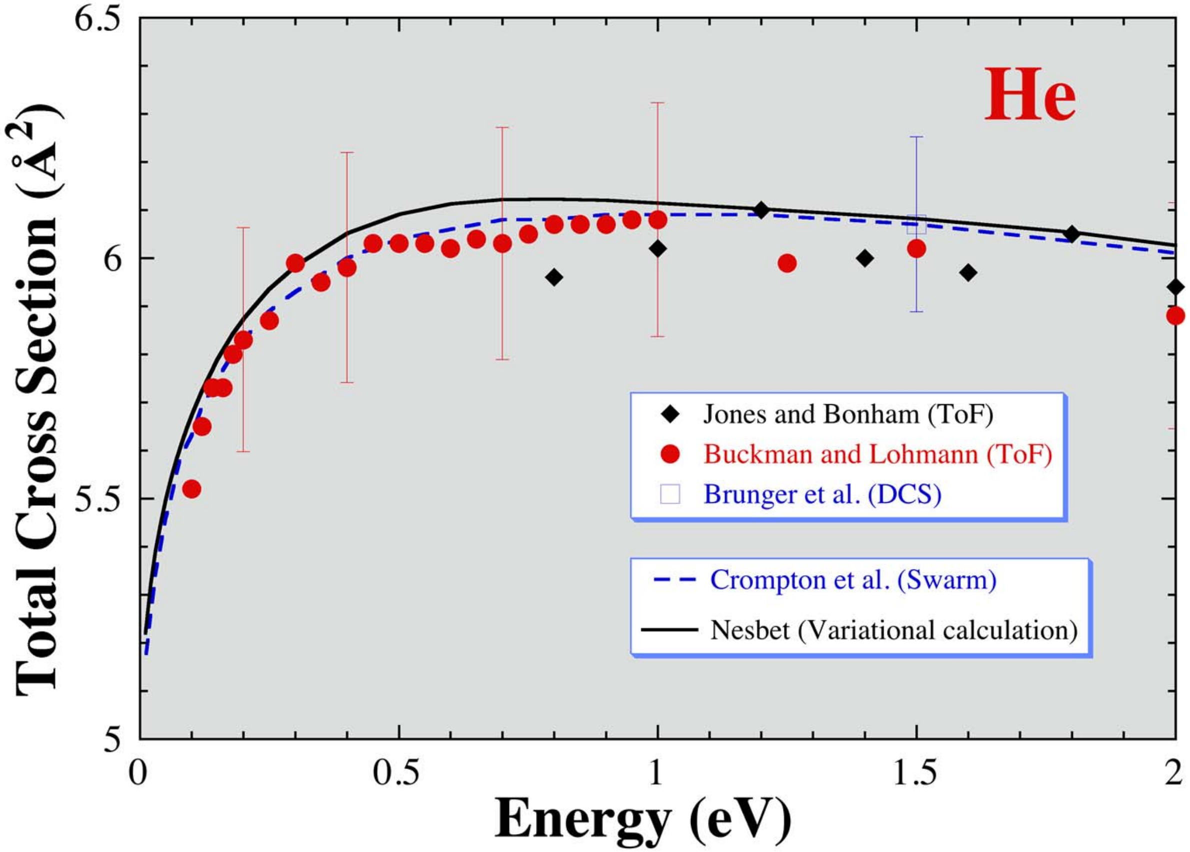
Why are they so different?

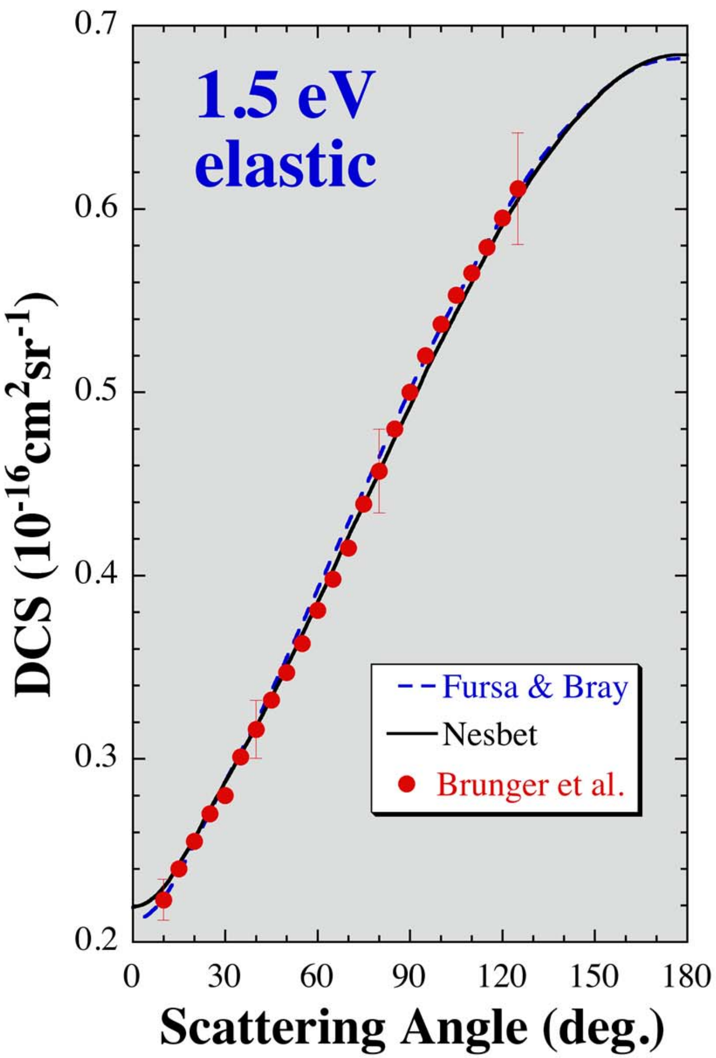
Ramsauer-Townsend minimum
- quantum effect

Heavy rare gases are transparent to low energy electrons !

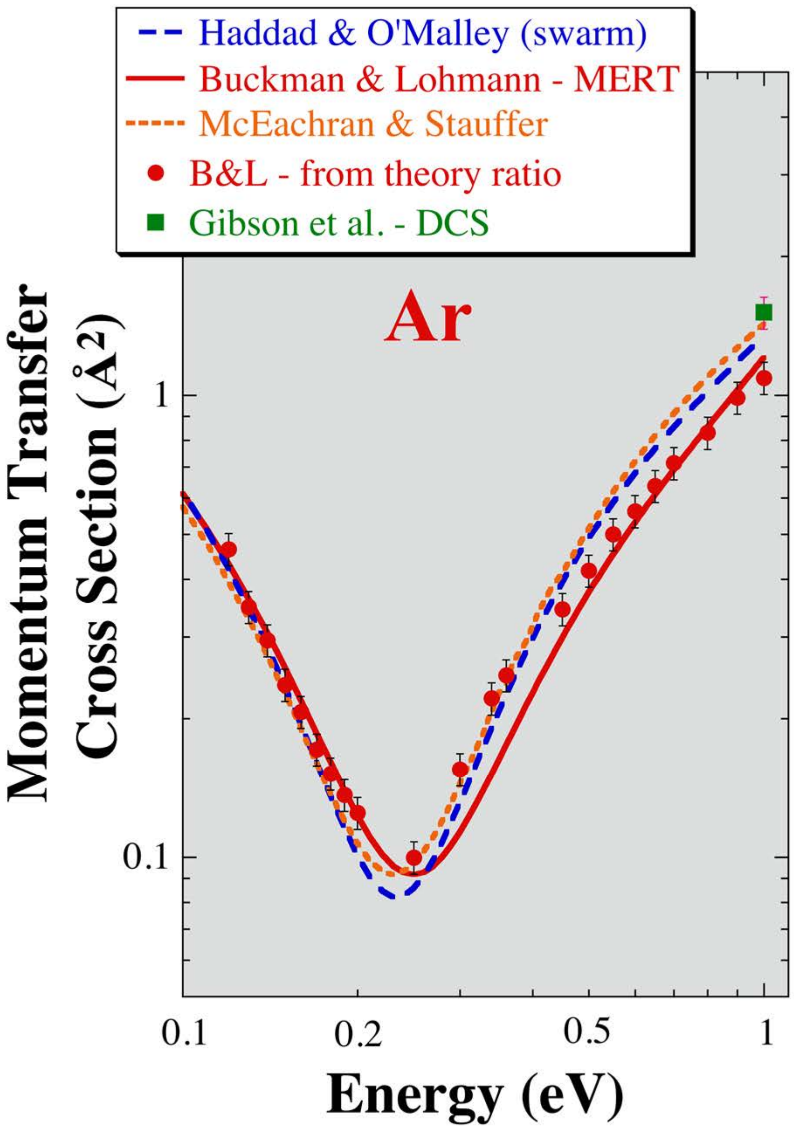


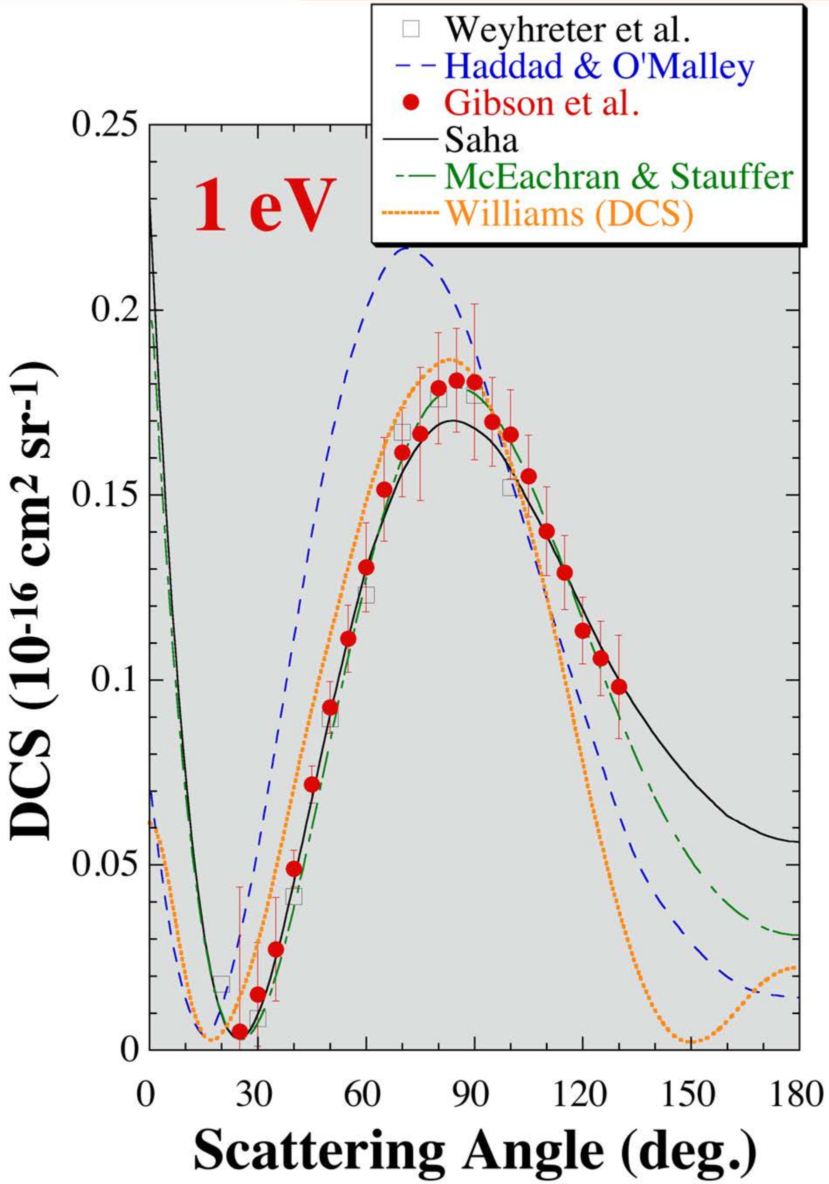
High Accuracy Elastic Scattering - Helium



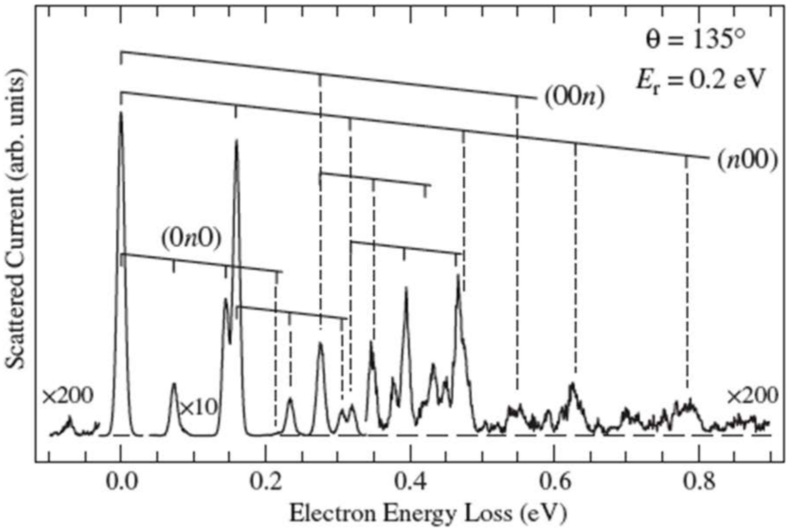


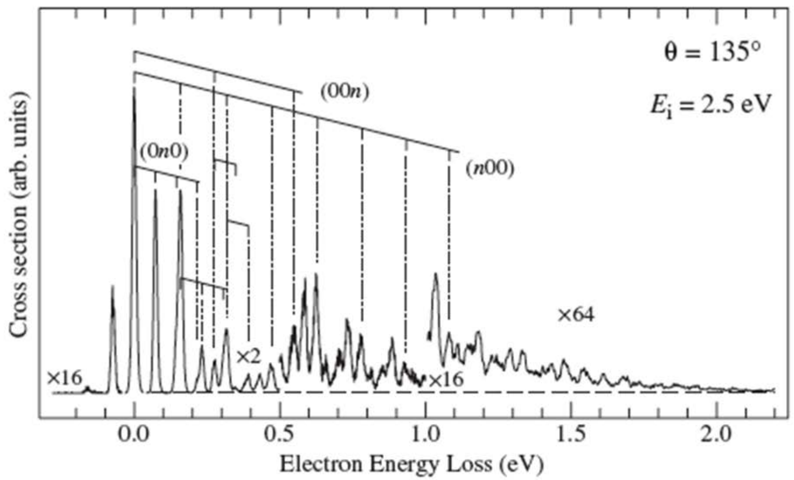
High Accuracy Elastic Scattering - Argon

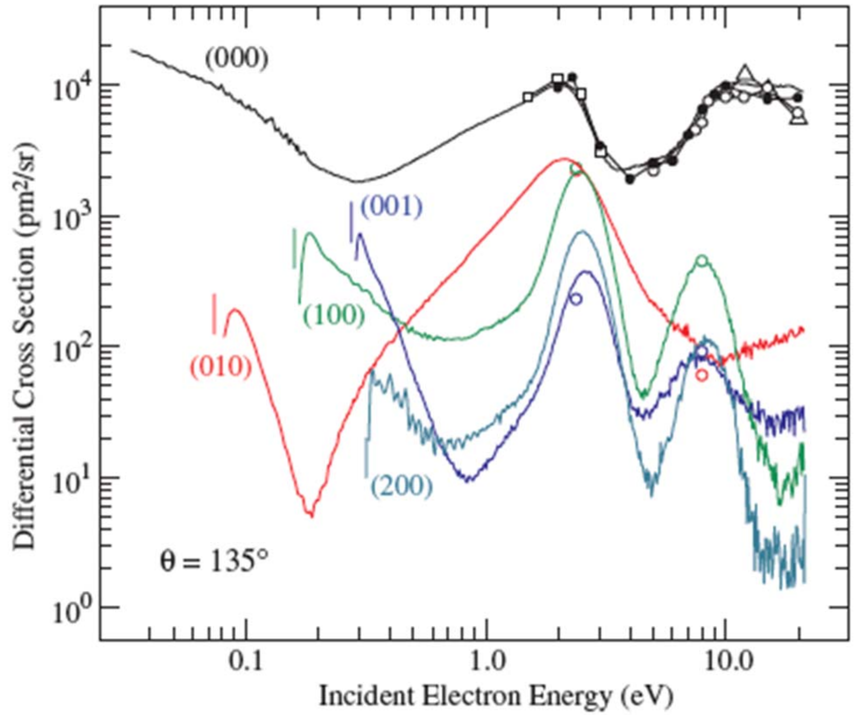




“State-of-the-Art” Measurements







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Resonance structure in low-energy electron scattering from OCS

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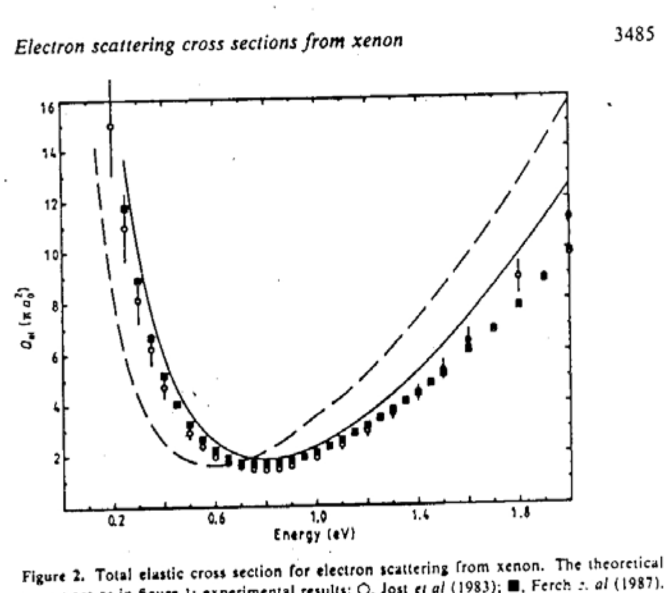
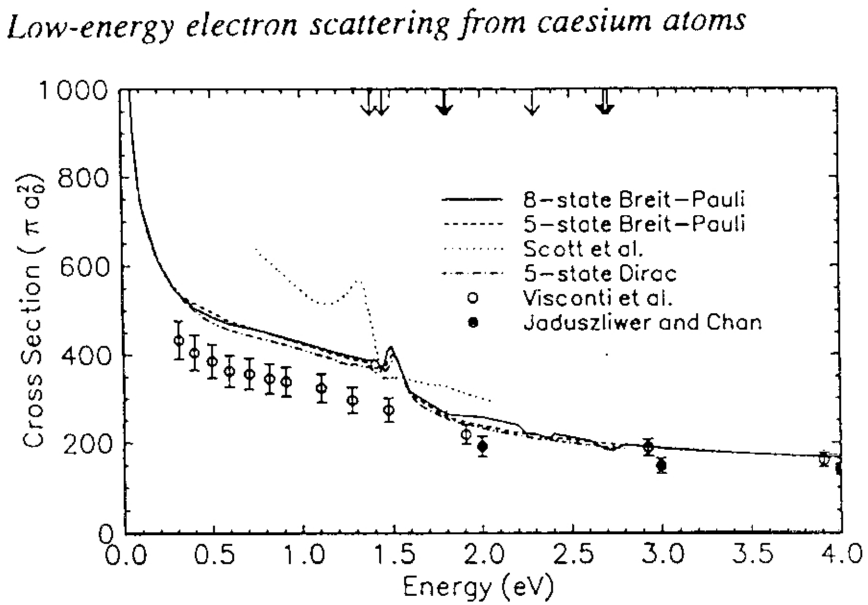
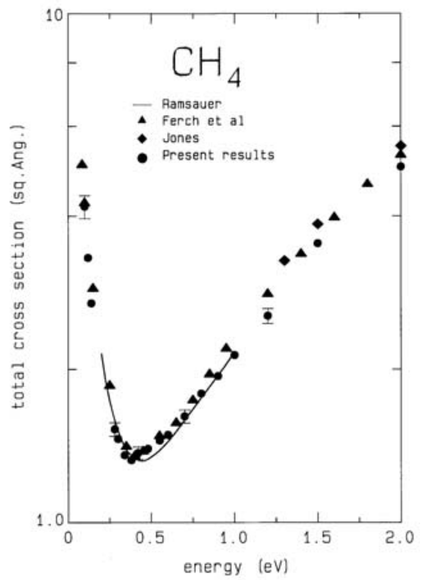
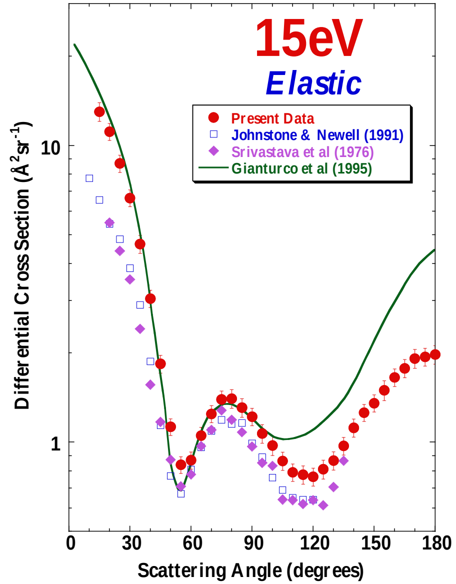
Cross Sections



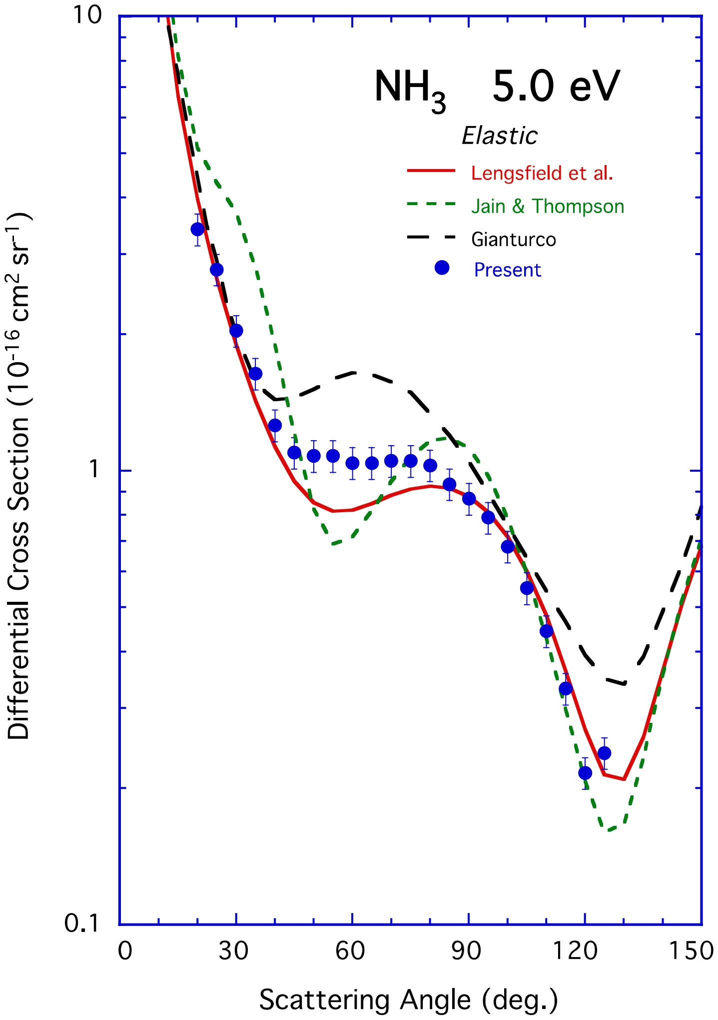


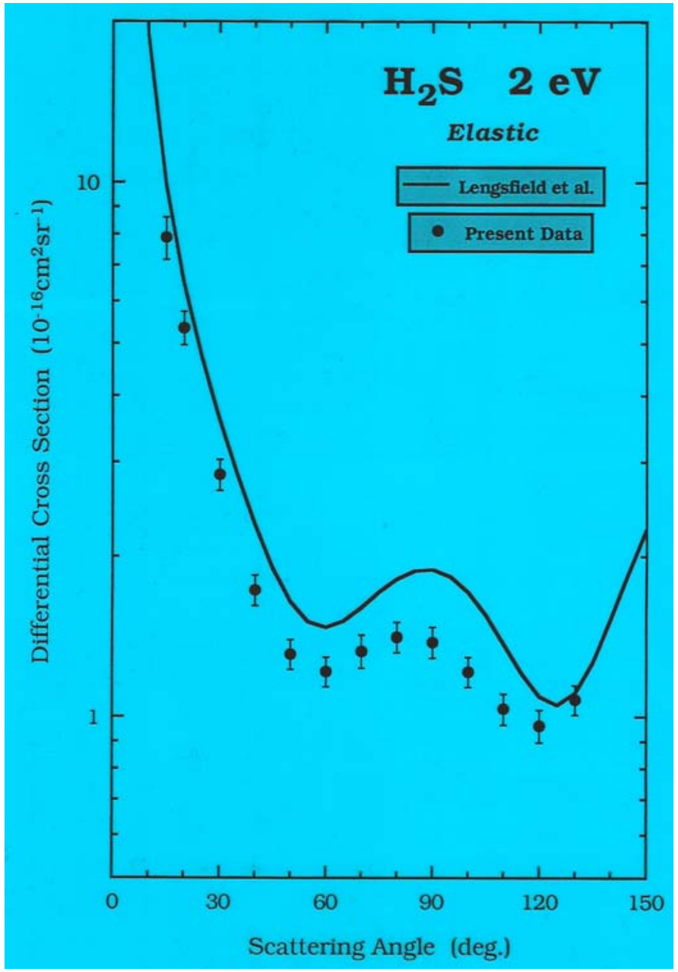
WHY SO DIFFERENT ???





Polar Molecules – strong scattering at small angles

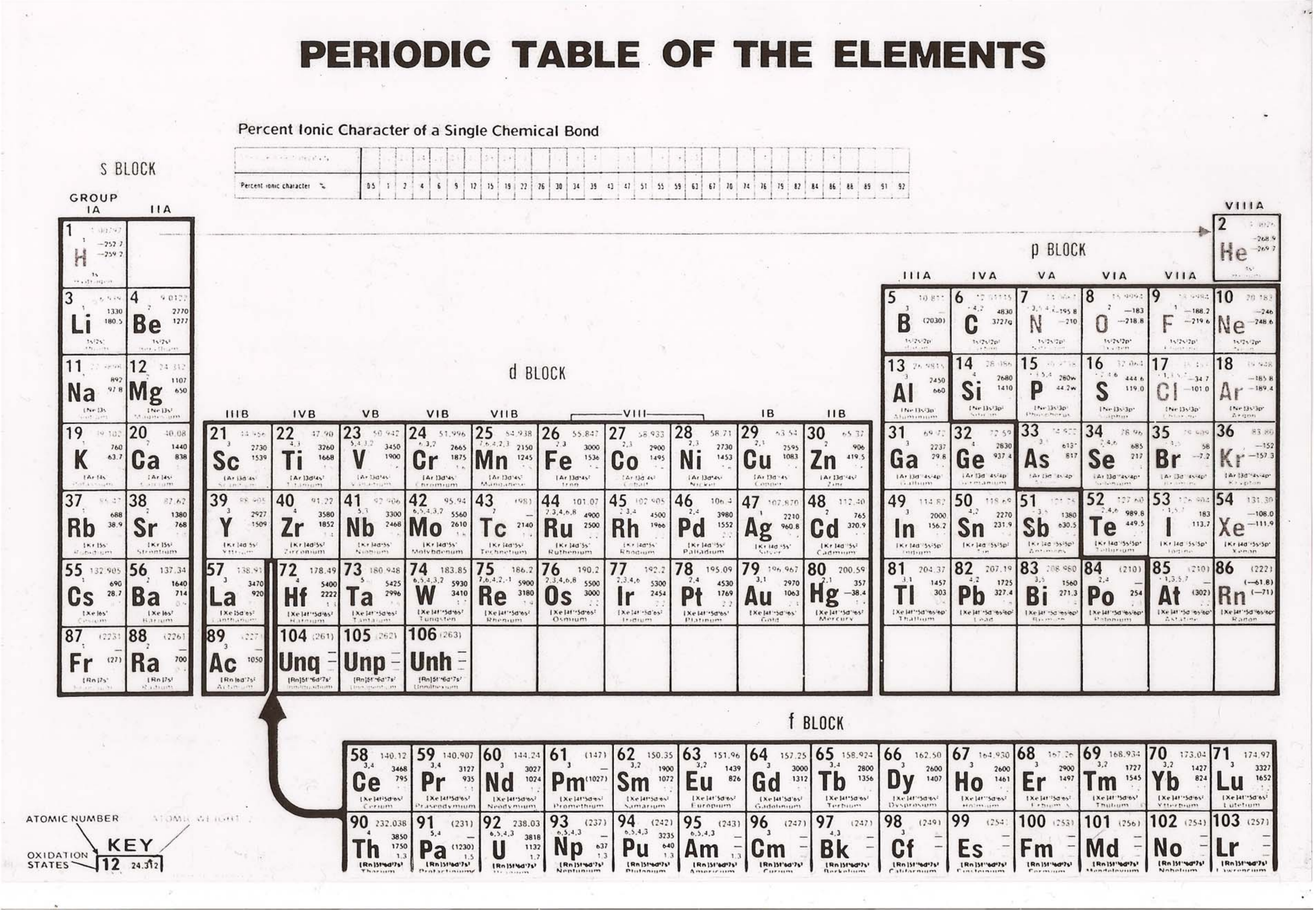




Atomic/Molecular Properties

- Atomic and Molecular Structure are KEY elements in Scattering
  - Binding Energies
  - Polarizabilities
  - Electron Affinities

The key to Structural Effects – Periodic Table



Binding Energies

Table 1.3. Electron configuration and ionization potentials I of atoms [1.1, 3]

Element	Electron configuration	Ground-state term	I [eV]	Element	Electron configuration	Ground state term	I [eV]
1 H	$1s$	$^2S_{1/2}$	13.598	52 Te	$5s^2 5p^4$	$^3P_2$	9.009
2 He	$1s^2$	$^1S_0$	24.587	53 I	$5s^2 5p^5$	$^2P_{3/2}$	10.451
3 Li	$1s^2 2s$	$^2S_{1/2}$	5.392	54 Xe	$5s^2 5p^6$	$^1S_0$	12.130
4 Be	$1s^2 2s^2$	$^1S_0$	9.322	55 Cs	$5p^6 6s$	$^2S_{1/2}$	3.894
5 B	$2s^2 2p$	$^2P_{1/2}$	8.298	56 Ba	$5p^6 6s^2$	$^1S_0$	5.212
6 C	$2s^2 2p^2$	$^3P_0$	11.260	57 La	$5d6s^2$	$^2D_{3/2}$	5.577
7 N	$2s^2 2p^3$	$^4S_{3/2}$	14.534	58 Ce	$4f5d6s^2$	$^1G_4$	5.47
8 O	$2s^2 2p^4$	$^3P_2$	13.618	59 Pr	$4f^3 6s^2$	$^4I_{9/2}$	5.42
9 F	$2s^2 2p^5$	$^2P_{3/2}$	17.422	60 Nd	$4f^4 6s^2$	$^5I_4$	5.49
10 Ne	$2s^2 2p^6$	$^1S_0$	21.564	61 Pm	$4f^5 6s^2$	$^6H_{5/2}$	5.55
11 Na	$2p^6 3s$	$^2S_{1/2}$	5.139	62 Sm	$4f^6 6s^2$	$^7F_0$	5.63
12 Mg	$2p^6 3s^2$	$^1S_0$	7.646	63 Eu	$4f^7 6s^2$	$^8S_{7/2}$	5.67
13 Al	$3s^2 3p$	$^2P_{1/2}$	5.986	64 Gd	$4f^7 5d6s^2$	$^9D_2$	6.14
14 Si	$3s^2 3p^2$	$^3P_0$	8.151	65 Tb	$4f^9 6s^2$	$^6H_{15/2}$	5.85
15 P	$3s^2 3p^3$	$^4S_{3/2}$	10.486	66 Dy	$4f^{10} 6s^2$	$^5I_8$	5.93
16 S	$3s^2 3p^4$	$^3P_2$	10.360	67 Ho	$4f^{11} 6s^2$	$^4I_{15/2}$	6.02
17 Cl	$3s^2 3p^5$	$^2P_{3/2}$	12.967	68 Er	$4f^{12} 6s^2$	$^3H_6$	6.10
18 Ar	$3s^2 3p^6$	$^1S_0$	15.759	69 Tm	$4f^{13} 6s^2$	$^2F_{7/2}$	6.18
19 K	$3p^6 4s$	$^2S_{1/2}$	4.341	70 Yb	$4f^{14} 6s^2$	$^1S_0$	6.254
20 Ca	$3p^6 4s^2$	$^1S_0$	6.113	71 Lu	$5d6s^2$	$^2D_{3/2}$	5.426
21 Sc	$3d4s^2$	$^2D_{3/2}$	6.54	72 Hf	$5d^2 6s^2$	$^3F_2$	7.0
22 Ti	$3d^2 4s^2$	$^3F_2$	6.82	73 Ta	$5d^3 6s^2$	$^4F_{3/2}$	7.89
23 V	$3d^3 4s^2$	$^4F_{3/2}$	6.74	74 W	$5d^4 6s^2$	$^5D_0$	7.98
24 Cr	$3d^5 4s$	$^7S_3$	6.766	75 Re	$5d^5 6s^2$	$^5S_{5/2}$	7.88
25 Mn	$3d^5 4s^2$	$^6S_{5/2}$	7.435	76 Os	$5d^6 6s^2$	$^5D_4$	8.7
26 Fe	$3d^6 4s^2$	$^5D_4$	7.870	77 Ir	$5d^7 6s^2$	$^4F_{9/2}$	9.1
27 Co	$3d^7 4s^2$	$^4F_{9/2}$	7.86	78 Pt	$5d^9 6s$	$^3D_3$	9.0
28 Ni	$3d^8 4s^2$	$^3F_4$	7.635	79 Au	$5d^{10} 6s$	$^2S_{1/2}$	9.225
29 Cu	$3d^{10} 4s$	$^2S_{1/2}$	7.726	80 Hg	$5d^{10} 6s^2$	$^1S_0$	10.437
30 Zn	$3d^{10} 4s^2$	$^1S_0$	9.394	81 Tl	$6s^2 6p$	$^2P_{1/2}$	6.108
31 Ga	$4s^2 4p$	$^2P_{1/2}$	5.999	82 Pb	$6s^2 6p^2$	$^3P_0$	7.416
32 Ge	$4s^2 4p^2$	$^3P_0$	7.899	83 Bi	$6s^2 6p^3$	$^4S_{3/2}$	7.289
33 As	$4s^2 4p^3$	$^4S_{3/2}$	9.81	84 Po	$6s^2 6p^4$	$^3P_2$	8.42
34 Se	$4s^2 4p^4$	$^3P_2$	9.752	85 At	$6s^2 6p^5$	$^2P_{3/2}$	9.5
35 Br	$4s^2 4p^5$	$^2P_{3/2}$	11.814	86 Rn	$6s^2 6p^6$	$^1S_0$	10.748
36 Kr	$4s^2 4p^6$	$^1S_0$	13.999	87 Fr	$6p^6 7s$	$^2S_{1/2}$	4.0
37 Rb	$4p^6 5s$	$^2S_{1/2}$	4.177	88 Ra	$6p^6 7s^2$	$^1S_0$	5.279
38 Sr	$4p^6 5s^2$	$^1S_0$	5.695	89 Ac	$6d7s^2$	$^2D_{3/2}$	5.170
39 Y	$4d5s^2$	$^2D_{3/2}$	6.38	90 Th	$6d^2 7s^2$	$^3F_2$	6.080
40 Zr	$4d^2 5s^2$	$^3F_2$	6.84	91 Pa	$5f^2 6d7s^2$	$^4K_{11/2}$	5.890
41 Nb	$4d^4 5s$	$^6D_{1/2}$	6.88	92 U	$5f^3 6d7s^2$	$^5L_6$	6.050
42 Mo	$4d^5 5s$	$^7S_3$	7.099	93 Np	$5f^4 6d7s^2$	$^6L_{11/2}$	6.190
43 Tc	$4d^5 5s^2$	$^6S_{5/2}$	7.28	94 Pu	$5f^6 7s^2$	$^7F_0$	6.062
44 Ru	$4d^7 5s$	$^5F_5$	7.37	95 Am	$5f^7 7s^2$	$^8S_{7/2}$	5.993
45 Rh	$4d^8 5s$	$^4F_{9/2}$	7.46	96 Cm	$5f^7 6d7s^2$	$^9D_2$	6.021
46 Pd	$4p^6 4d^{10}$	$^1S_0$	8.34	97 Bk	$5f^9 7s^2$	$^6H_{15/2}$	6.229
47 Ag	$4d^{10} 5s$	$^2S_{1/2}$	7.576	98 Cf	$5f^{10} 7s^2$	$^5I_8$	6.298
48 Cd	$4d^{10} 5s^2$	$^1S_0$	8.993	99 Es	$5f^{11} 7s^2$	$^4I_{15/2}$	6.422
49 In	$5s^2 5p$	$^2P_{1/2}$	5.786	100 Fm	$5f^{12} 7s^2$	$^3H_6$	6.500
50 Sn	$5s^2 5p^2$	$^3P_0$	7.344	101 Md	$5f^{13} 7s^2$	$^2F_{7/2}$	6.580
51 Sb	$5s^2 5p^3$	$^4S_{3/2}$	8.641	102 No	$5f^{14} 7s^2$	$^1S_0$	6.650

From V.P. Shevelko
‘Atoms and Their Spectroscopic Properties
Springer

Examples of the Binding Energies (ionization Potentials) for some atoms (in eV) are:

H	13.6	He	24.6
Li	5.4	Ne	21.6
Na	5.1	Ar	15.8
K	4.34	Kr	14.0
Rb	4.2	Xe	12.1
Cs	3.9	Rn	10.7

Table 1 (continued)
FORMULA INVOLVING POLARIZABILITY

Description	Formula	Remarks
Rayleigh scattering cross section	$\sigma(\nu) = \left(\frac{8\pi}{9c^4}\right)(2\pi\nu)^4 \times \left[3\alpha^2(\nu) + \frac{2}{3}\gamma^2(\nu)\right]$	The photon frequency is ν; the average polarizability is $\alpha(\nu)$ and the polarizability anisotropy (the difference between polarizabilities parallel and perpendicular to the applied field) is $\gamma(\nu)$
Verdet constant	$V(\nu) = \frac{\nu n}{2mc^2}\left(\frac{d\alpha(\nu)}{d\nu}\right)$	Defined from $\theta = V(\nu)B$, where θ is the angle of rotation of linearly polarized light through a medium of number density n, per unit length, for a longitudinal magnetic field strength B (Faraday effect)

Table 2
STATIC AVERAGE ELECTRIC DIPOLE POLARIZABILITIES FOR GROUND STATE ATOMS

Atomic Number	Atom	Polarizability (units of 10^{-24} cm^3)	Estimated accuracy (%)	Method	Ref.
1	H	0.666793	"exact"	Calc	MB77
2	He	0.204956	"exact"	Calc	MB77
		0.2050	0.1	Index/diel	NB65/OC67
3	Li	24.3	2	Beam	MB77
4	Be	5.60	2	Calc	MB77
5	B	3.03	2	Calc	MB77
6	C	1.76	2	Calc	MB77
7	N	1.10	2	Calc/index	MB77
8	O	0.802	2	Calc/index	MB77
9	F	0.557	2	Calc	MB77
10	Ne	0.3956	0.1	Diel	OC67
11	Na	23.6	2	Beam	MB77
12	Mg	10.6	2	Calc	MB77
13	Al	8.34	2	Calc	MB77
14	Si	5.38	2	Calc	MB77
15	P	3.63	2	Calc	MB77
16	S	2.90	2	Calc	MB77
17	Cl	2.18	2	Calc	MB77
18	Ar	1.6411	0.05	Index/diel	NB65/OC67
19	K	43.4	2	Beam	MB77
20	Ca	22.8	2	Calc	MB77
		25.0	8	Beam	MB77
21	Sc	17.8	25	Calc	D84
22	Ti	14.6	25	Calc	D84
23	V	12.4	25	Calc	D84
24	Cr	11.6	25	Calc	D84
25	Mn	9.4	25	Calc	D84
26	Fe	8.4	25	Calc	D84
27	Co	7.5	25	Calc	D84
28	Ni	6.8	25	Calc	D84
29	Cu	6.1	25	Calc	D84
		7.31	25	Calc	G84
30	Zn	7.1	25	Calc	MB77
		5.6	25	Calc	D84
31	Ga	8.12	2	Calc	MB77
32	Ge	6.07	2	Calc	MB77
33	As	4.31	2	Calc	MB77
34	Se	3.77	2	Calc	MB77
35	Br	3.05	2	Calc	MB77
36	Kr	2.4844	0.05	Diel	OC67
37	Rb	47.3	2	Beam	MB77
38	Sr	27.6	8	Beam	MB77
39	Y	22.7	25	Calc	D84
40	Zr	17.9	25	Calc	D84
41	Nb	15.7	25	Calc	D84
42	Mo	12.8	25	Calc	D84
43	Tc	11.4	25	Calc	D84
44	Ru	9.6	25	Calc	D84
45	Rh	8.6	25	Calc	D84
46	Pd	4.8	25	Calc	D84
47	Ag	7.2	25	Calc	D84
		8.56	25	Calc	G84
48	Cd	7.2	25	Calc	D84

Table 2 (continued)
STATIC AVERAGE ELECTRIC DIPOLE POLARIZABILITIES FOR GROUND STATE ATOMS

Atomic Number	Atom	Polarizability (units of 10^{-24} cm^3)	Estimated accuracy (%)	Method	Ref.
49	In	10.2	12	Beam	GMBSJ84
		9.1	25	Calc	D84
50	Sn	7.7	25	Calc	D84
51	Sb	6.6	25	Calc	D84
52	Te	5.5	25	Calc	D84
53	I	5.35	25	Index	A56
		4.7	25	Calc	D84
54	Xe	4.044	0.5	Diel	MB77
55	Cs	59.6	2	Beam	MB77
56	Ba	39.7	8	Beam	MB77
57	La	31.1	25	Calc	D84
58	Ce	29.6	25	Calc	D84
59	Pr	28.2	25	Calc	D84
60	Nd	31.4	25	Calc	D84
61	Pm	30.1	25	Calc	D84
62	Sm	28.8	25	Calc	D84
63	Eu	27.7	25	Calc	D84
64	Gd	23.5	25	Calc	D84
65	Tb	25.5	25	Calc	D84
66	Dy	24.5	25	Calc	D84
67	Ho	23.6	25	Calc	D84
68	Er	22.7	25	Calc	D84
69	Tm	21.8	25	Calc	D84
70	Yb	21.0	25	Calc	D84
71	Lu	21.9	25	Calc	D84
72	Hf	16.2	25	Calc	D84
73	Ta	13.1	25	Calc	D84
74	W	11.1	25	Calc	D84
75	Re	9.7	25	Calc	D84
76	Os	8.5	25	Calc	D84
77	Ir	7.6	25	Calc	D84
78	Pt	6.5	25	Calc	D84
79	Au	5.8	25	Calc	D84
		6.48	25	Calc	G84
80	Hg	5.7	25	Calc	D84
		5.1	15	Diel	MB77
81	Tl	7.6	15	Beam	NYU84
		7.5	25	Calc	D84
82	Pb	6.8	25	Calc	D84
83	Bi	7.4	25	Calc	D84
84	Po	6.8	25	Calc	D84
85	At	6.0	25	Calc	D84
86	Rn	5.3	25	Calc	D84
87	Fr	48.7	25	Calc	D84
88	Ra	38.3	25	Calc	D84
89	Ac	32.1	25	Calc	D84
90	Th	32.1	25	Calc	D84
91	Pa	25.4	25	Calc	D84
92	U	27.4	25	Calc	D84
93	Np	24.8	25	Calc	D84
94	Pu	24.5	25	Calc	D84
95	Am	23.3	25	Calc	D84
96	Cm	23.0	25	Calc	D84
97	Bk	22.7	25	Calc	D84
98	Cf	20.5	25	Calc	D84
99	Es	19.7	25	Calc	D84
100	Fm	23.8	25	Calc	D84
101	Md	18.2	25	Calc	D84
102	No	17.5	25	Calc	D84

Note: Calc = calculated value; Beam = atomic beam deflection technique; Index = determination based on the measured index of refraction; Diel = determination based on the measured dielectric constant.

REFERENCES

A56. **Atoji, M.,** *J. Chem. Phys.*, 25, 174, 1956. Semiempirical method based on molecular polarizabilities and atomic radii.

D84. **Doolen, G. D.,** Los Alamos National Laboratory, unpublished. A relativistic linear response method was used. The method is that described by A. Zangwill and P. Soven, *Phys. Rev. A*, 21, 1561, 1980. Adjustments of less than 10% have been made to these results to bring them into agreement with accurate experimental values where available, for the purpose of presenting "recommended" polarizabilities in Table 2. (T. M. Miller.)

G84 **Gollisch, H.,** *J. Phys. B*, 17, 1463, 1984. Other results and useful references are contained in this paper.

GMBSJ84. **Guella, T. P., Miller, T. M., Bederson, B., Stockdale, J. A. D., and Jaduszliwer, B.,** *Phys. Rev. A*, 29, 2977, 1984.

Binding Energies and Polarizabilities

Examples of the Binding Energies (ionization Potentials) for some atoms (in eV) are:

H	13.6	He	24.6
Li	5.4	Ne	21.6
Na	5.1	Ar	15.8
K	4.3	Kr	14.0
Rb	4.2	Xe	12.1
Cs	3.9	Rn	10.7

Examples of the dipole polarizabilities for some atoms (in units of a_0^3) are

H	4.5	H^-	206	He	1.38
Li	165	Li^-	750	Ne	2.66
		(Li^+	0.2)		
Na	160			Ar	11.08
K	290			Kr	16.8
Rb	320			Xe	27.3
Cs	403				

Electron Affinities

Table 1.5. Electron affinities I

Nuclear charge Z	Ion, term	Configuration	I [eV]
1	$D^-(^1S)$	$1s^2$	0.754593
1	$H^-(^1S)$	$1s^2$	0.754202
2	$He^-(^4P)$	$1s2s2p$	0.077
3	$Li^-(^1S)$	$1s^22s^2$	0.6180
	$Li^-(^3P)$	$2s2p^2$	0.050
4	$Be^-(^4P)$	$2s2p^2$	0.291
	$Be^-(^4S)$	$1s^22p^3$	0.295
5	$B^-(^3P)$	$2s^22p^2$	0.277
	$B^-(^1P)$	$2s^22p^2$	0.104
6	$C^-(^4S^0)$	$2s^22p^3$	1.2629
	$C^-(^2D)$	$2s^22p^3$	0.035
7	$N^-(^3P)$	$2s^22p^4$	0.2–0.7
8	$O^-(^2P)$	$2s^22p^5$	1.4611103
9	$F^-(^1S)$	$2s^22p^6$	3.401190
11	$Na^-(^1S)$	$3s^2$	0.547926
13	$Al^-(^3P_0)$	$3p^2$	0.441
	$Al^-(^1D_2)$	$3p^2$	0.33
14	$Si^-(^4S)$	$3p^3$	1.389
	$Si^-(^2D)$	$3p^3$	0.526
	$Si^-(^2P_2)$	$3p^3$	0.034
15	$P^-(^3P)$	$3p^4$	0.7465
16	$S^-(^2P)$	$3p^5$	2.077104
17	$Cl^-(^1S)$	$3p^6$	3.61269
19	$K^-(^1S)$	$4s^2$	0.50147
20	$Ca^-(^2P_{1/2})$	$4s^24p$	0.0175–0.0246
	$Ca^-(^2P_{3/2})$	$4s^24p$	0.0197
21	$Se^-(^1D)$	$3d4s^24p$	0.188
	$Se^-(^3D)$	$3d4s^24p$	0.04
22	$Ti^-(^4F)$	$3d^34s^2$	0.079
23	$V^-(^5D)$	$3d^44s^2$	0.525
24	$Cr^-(^6S)$	$3d^54s^2$	0.666
26	$Fe^-(^4F)$	$3d^74s^2$	0.151
27	$Co^-(^3F)$	$3d^84s^2$	0.662
28	$Ni^-(^2D)$	$3d^94s^2$	1.156
29	$Cu^-(^1S)$	$3d^{10}4s^2$	1.235
31	$Ga^-(^3P)$	$4p^2$	0.3
32	$Ge^-(^4S)$	$4p^3$	1.233
33	$As^-(^3P)$	$4p^4$	0.81
34	$Se^-(^2P)$	$4p^5$	2.020670
35	$Br^-(^1S)$	$4p^6$	3.363590
37	$Rb^-(^1S)$	$5s^2$	0.48592
38	$Sr^-(^2P_{1/2})$	$5s^25p$	0.054
	$Sr^-(^2P_{3/2})$	$5s^25p$	0.029
39	$Y^-(^1D)$	$4d5s^25p$	0.307
	$Y^-(^3D)$	$4d5s^25p$	0.16
40	$Zr^-(^4F)$	$4d^35s^2$	0.426
41	$Nb^-(^5D)$	$4d^45s^2$	0.893
42	$Mo^-(^6S)$	$4d^55s^2$	0.746
43	$Tc^-(^5D)$	$4d^65s^2$	0.55
44	$Ru^-(^4F)$	$4d^75s^2$	1.05

WHAT ABOUT THE 'OTHER SIDE' OF THE PERIODIC TABLE?

GROUPS 6-7

They have a high affinity for electrons

How does this effect scattering?

e.g. O^- 1.46 eV

F^- 3.40 eV

Some general observations

There are significant differences in the energy dependence and absolute magnitude of total cross sections for low energy electron scattering from atoms and molecules

- Low energy collisions are dominated by outer electronic structure
- Collisions probe and reflect this structure

e.g. Compare Argon and Potassium atoms

– Ar (Z=18) $1s^2 2s^2 2p^6 3s^2 3p^6$ $\sigma_T(1\ eV) \approx 1$ Sq. Ang. $\alpha = 11.08\ a_o^{\ 3}$

– K (Z=19) $1s^2 2s^2 2p^6 3s^2 3p^6 4s$ $\sigma_T(1\ eV) \approx 350$ Sq. Ang. $\alpha = 293\ a_o^{\ 3}$

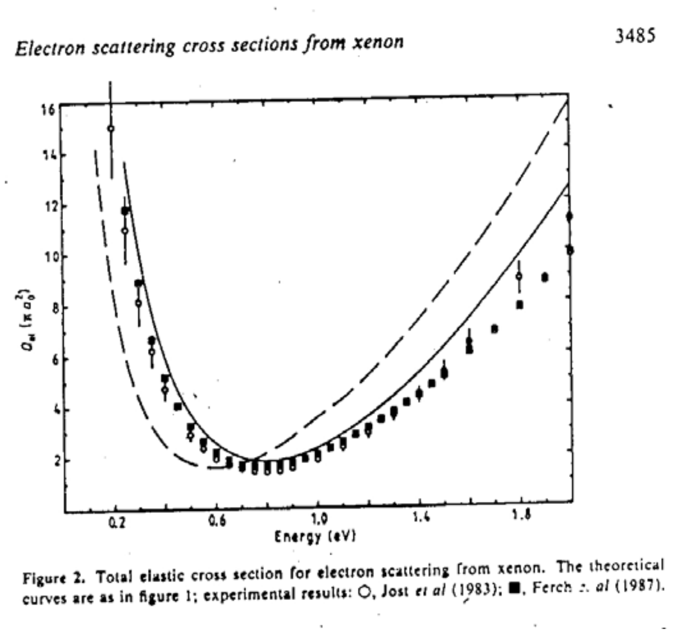
–e.g. Compare He and He(2^3S)

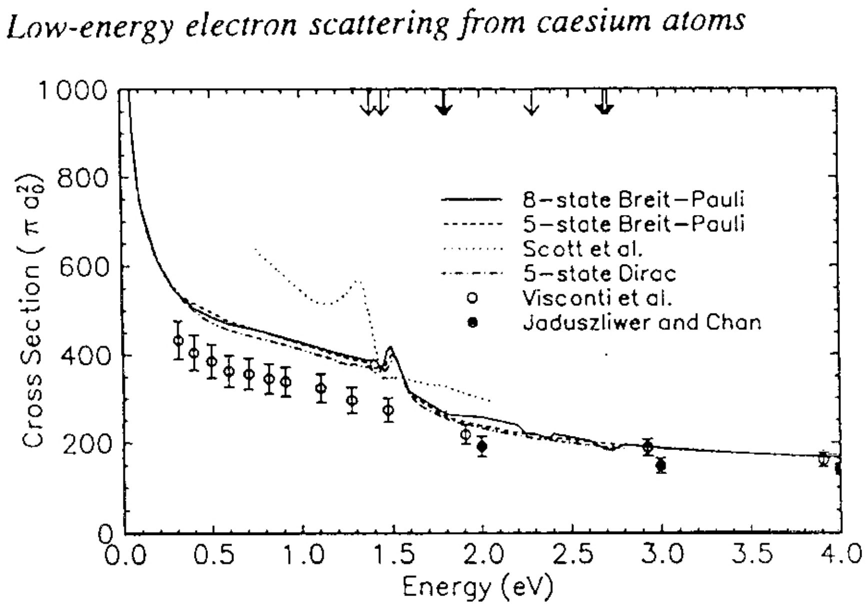
– He (Z=2) $1s^2\ {}^1S$ $\sigma_T(1\ eV) \approx 5$ Sq. Ang. $\alpha = 1.38\ a_o^{\ 3}$

– He* (Z=2) $1s2s\ {}^3S$ $\sigma_T(1\ eV) \approx 1000$ Sq. Ang. $\alpha \cong 350\ a_o^{\ 3}$

Atomic Structure is the dominant determinant of Scattering probability

Xe and Cs Comparison





α = 27.3 a.u.

α = 403 a.u.

R-T minimum

Scattering Resonances

Resonant Scattering in Atomic Physics

•A 'Resonant State' is a very common occurrence in low energy atomic physics – particularly electron scattering where they are also referred to as 'compound states' or 'temporary negative ions' or 'non-stationary' states

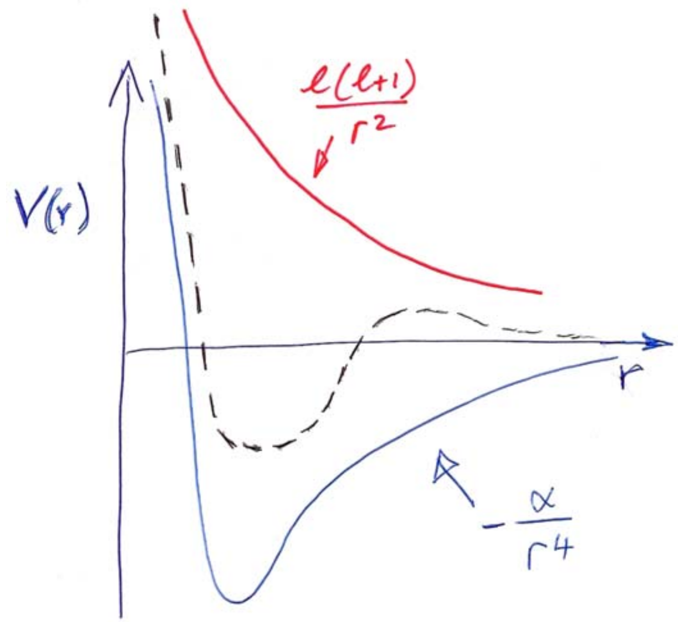
• $e^- + AB \rightarrow AB^- \rightarrow$?????

•ALL atoms and molecules support resonance states when low energy electron interact with them. They come in two principle types

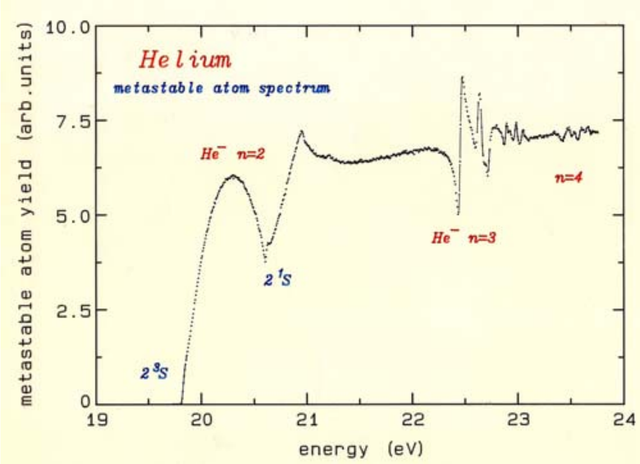
•**SHAPE RESONANCES and FESHBACH RESONANCES**

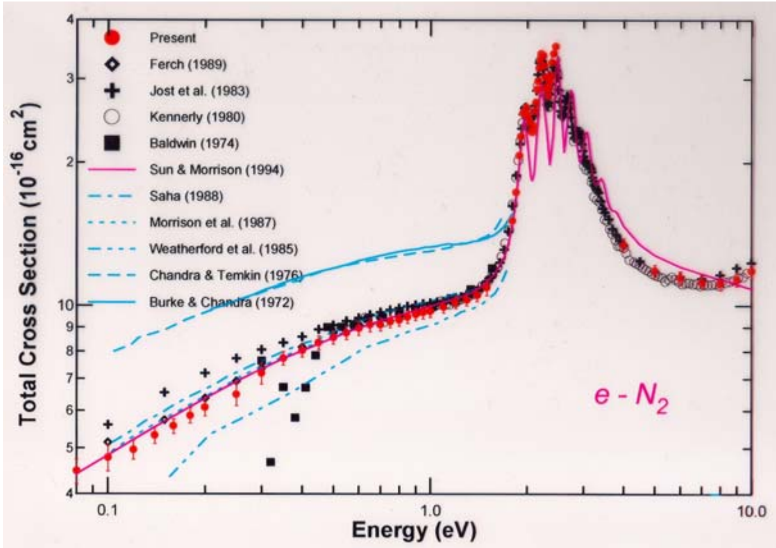
•**SHAPE RESONANCE**

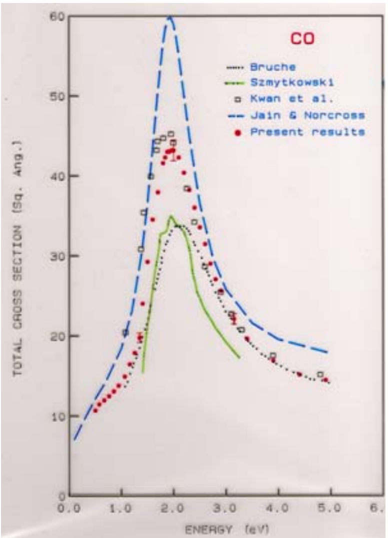
•The classical idealisation of a shape resonance depicts the projectile tunneling through a potential barrier, being confined or trapped within this barrier for the lifetime of the resonance, and then tunneling out again. The barrier is formed through a combination of the repulsive centrifugal potential and the attractive atomic mean field. Such a barrier is a property of the unperturbed atom.

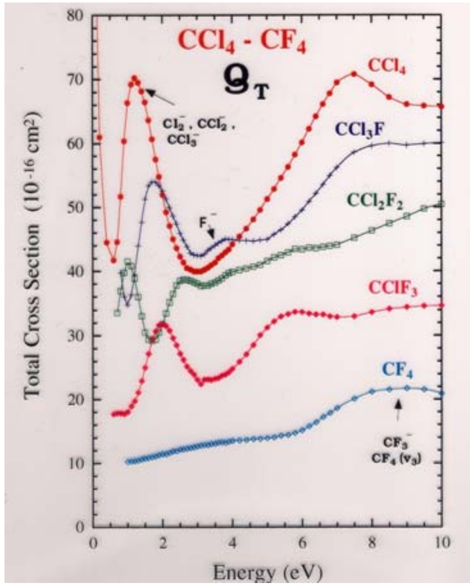


Resonant Scattering





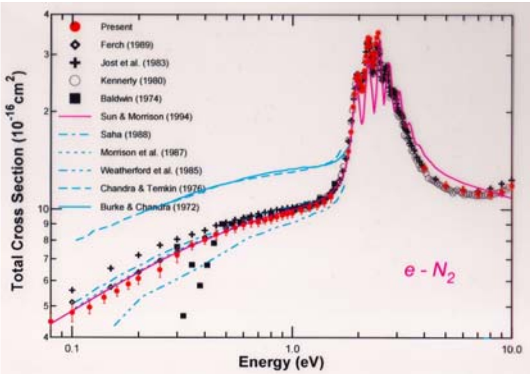




SOME EXAMPLES OF RESONANT SCATTERING

Shape Resonances

$$e^- + N_2(^1\Sigma) \rightarrow N_2^-(^2\Pi) \rightarrow e'^- + N_2{}^*(^1\Sigma)$$



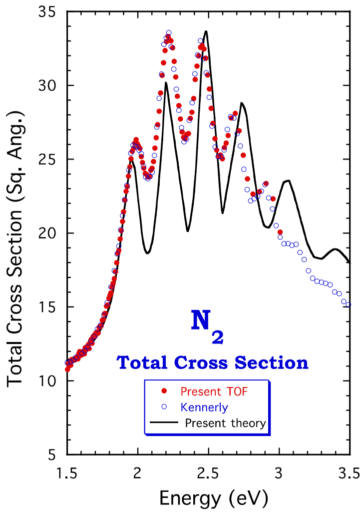
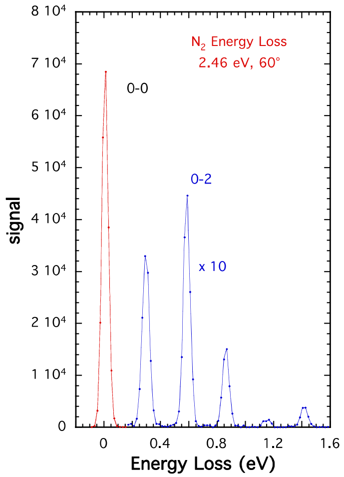


Figure 10(b)



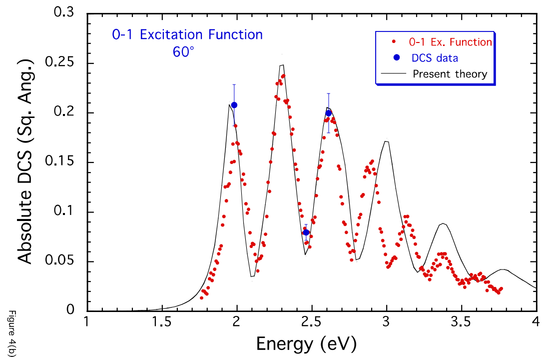


Figure 4(b)

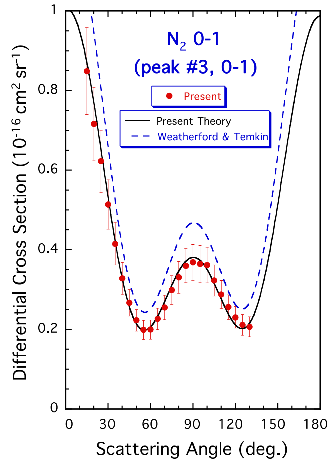


Figure 5(c)

Shape resonance in N_2
- occurs solely in the l=2 partial wave
- solely responsible for vibrational excitation in the N_2 molecule
- key role in a number of important technologies

Shape Resonances in Atoms

- e.g. Mercury
- Ground configuration of atom
  $6s^2\ {}^1S$
- Ground configuration of negative ion
  $6s^2\ 6p$
- Excited states of Negative ion
  $6s\ 6p^2$ etc……

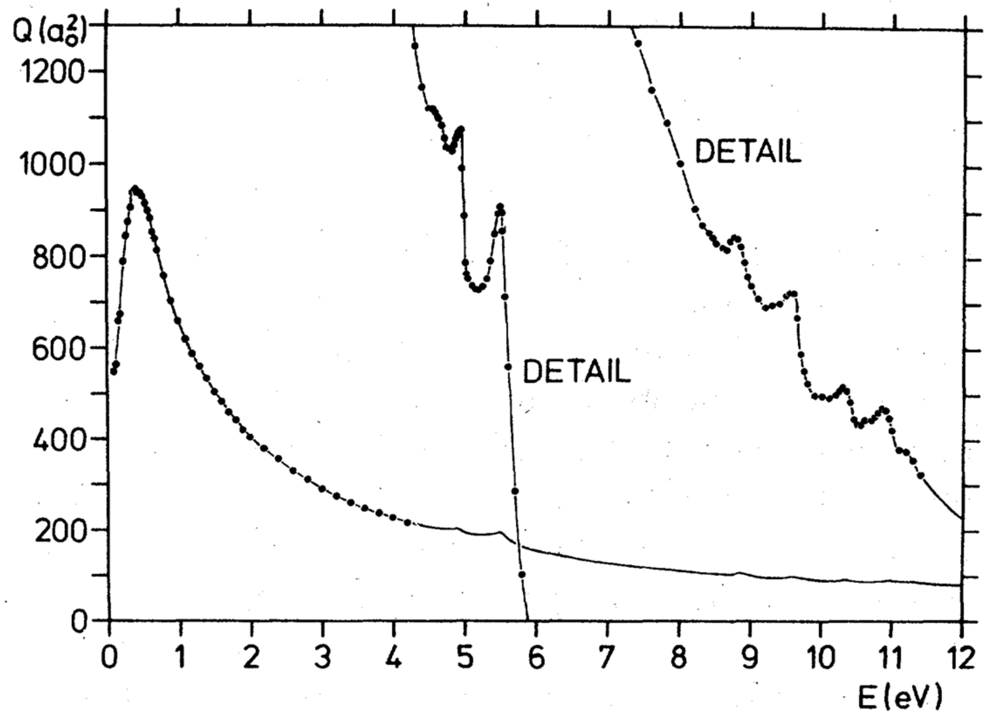


FIG. 11. Resonance structure of present results. Ordinate of details 25 ×enlarged; zero suppressed by $160a_0^2$ and $70a_0^2$, respectively.

Scattering Resonances

A **Feshbach** resonance involves the capture of the projectile via the deposition of its energy into some internal degree of freedom of the target, and its subsequent release when it re-acquires enough energy to escape.

In contrast to the mechanism for formation of a shape resonance, which is generally due to properties of the parent atom, a Feshbach resonance in an N-electron atom is an excited state of the N+1 electron complex – ie the negative ion, and it has its own dynamics which are distinct from those of the target. They typically form by the projectile being bound to, or in, the potential associated with an excited state of the atom.

•Thus Feshbach resonances often represent doubly excited states of the negative ion and they typically lie below their parent state in energy

•A Classic example occurs in the He atom

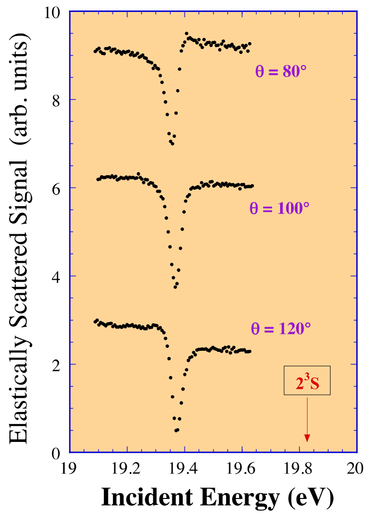
$$e^- + He(1s^2\ {}^1S) \rightarrow He^-(1s2s^2\ {}^2S) \rightarrow e^- + He(1s^2\ {}^1S)$$

This resonance state

- lies ~0.5 eV below its parent state (He 1s2s ^{3}S)

- can only be seen in the elastic channel

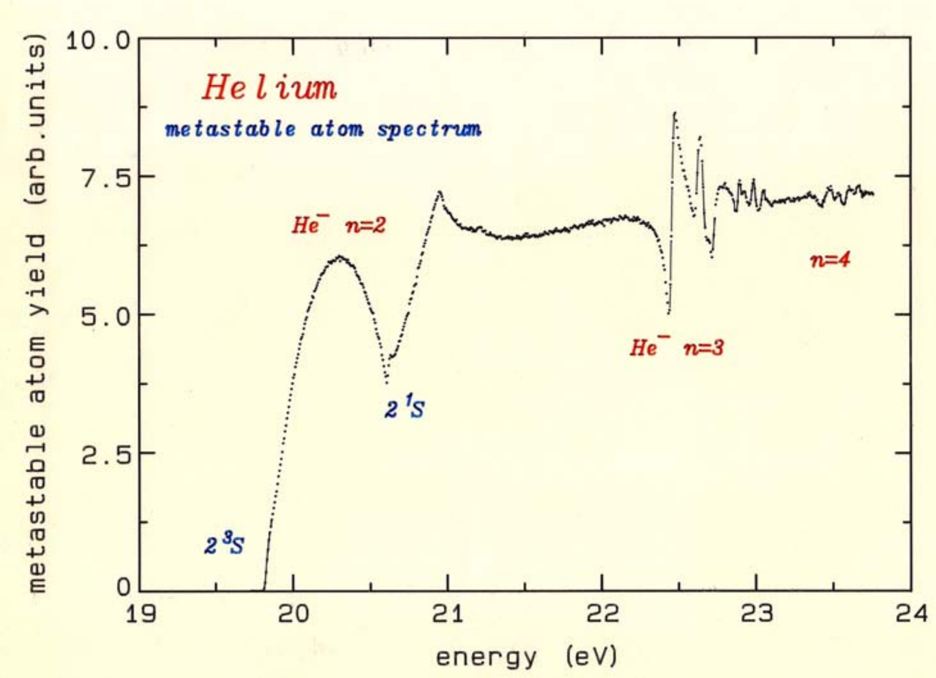
- has a long lifetime (narrow width)



Feshbach Resonances

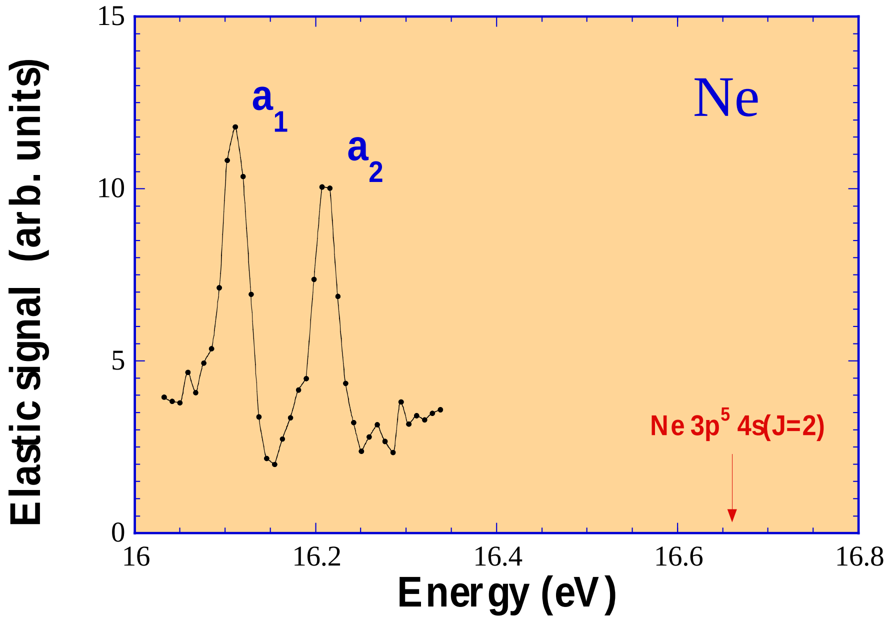
Higher lying states in He⁻

$$e^- + He(1s^2\ {}^1S) \rightarrow He^-(1snl\ n'l'\ {}^{1,2,3}L)$$
$$\rightarrow e'^- + He(1s2s\ {}^3S)$$



Heavier Rare Gases

$$e^- + Ne(3p^6\ {}^1S) \rightarrow Ne^-[2p^5\ {}^2P_{1/2,3/2}]3s^2\ {}^1S$$
$$\rightarrow e^- + Ne(3p^6\ {}^1S)$$



Resonances & Electron-Induced Chemistry

Transient negative ion formation at low Energies

$$e^- + AB \longrightarrow AB^-$$

'scattering'

'fragmentation'

$$AB^- \longrightarrow AB^* + e^-$$

Vibrational excitation
Electronic excitation
Elastic scattering

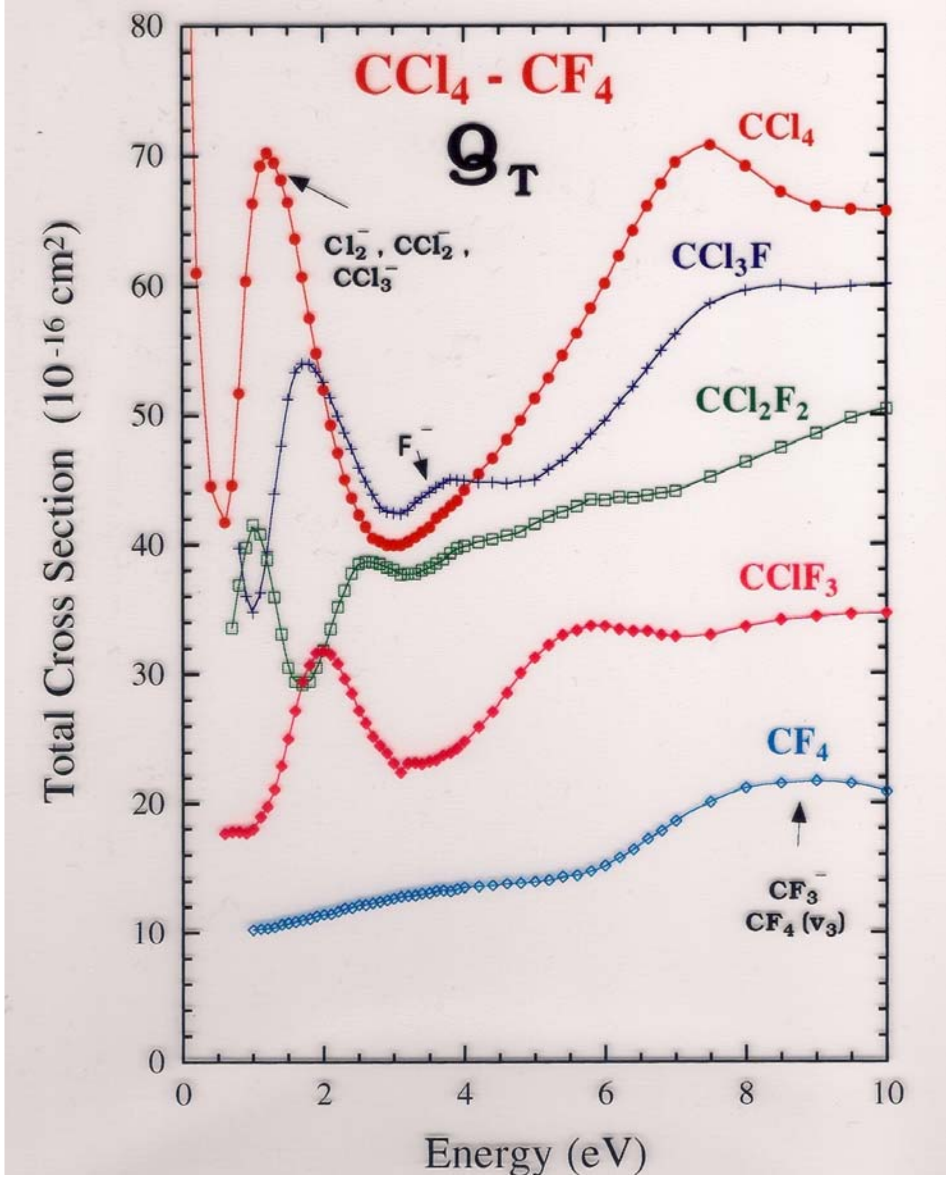
$$AB^- \longrightarrow A + B^-$$

Dissociative Attachment
Free radical formation

The chemistry proceeds preferentially because of the intermediate, transient (10^{-14}-10^{-12} sec) negative ion

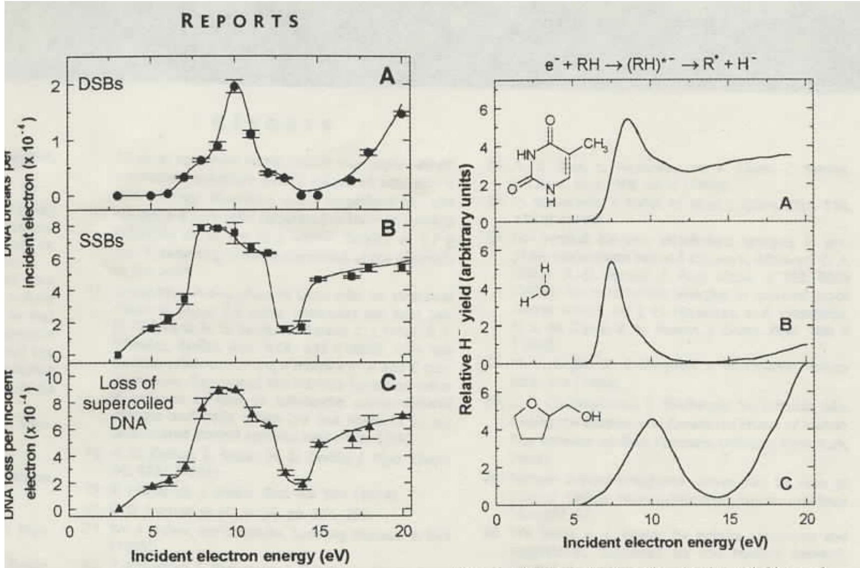
Resonances & Electron-Induced Chemistry

- Resonances in CxHy
  - often lead to dissociation via DEA
  - negative ions + neutrals
  - radical species
- Active etching species



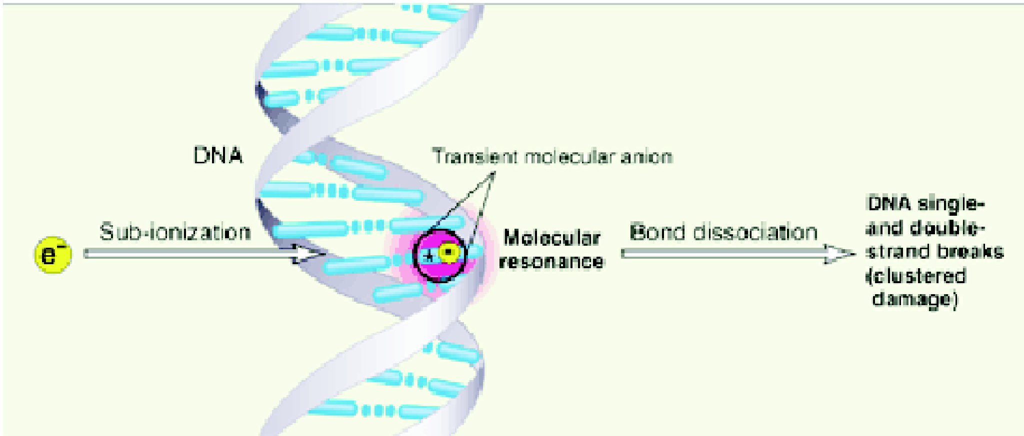
Electron-induced DNA strand breaks

Boudaiffa, Cloutier, Hunting, Huels & Sanche
Science 287 1658 (2000)



amage was performed using the ImageQuant program determined from linear least-squares fits to the initial ›onse curves (in the very low exposure, linear-response r supercoiled DNA loss and production of nicked circle). Each data point corresponds to an average of about easurements (each consisting of 8 to 12 DNA samples, ›osures). The error bars correspond to one standard cibility, of the measurement. Comparison of control samples held under UHV conditions, for equal time ›ry of plasmid DNA introduces only small amounts of ›able DSBs.

Fig. 2. Electron damage to condensed films of molecules RH = thymine (**A**), water (**B**), and tetrahydrofurfuryl alcohol (**C**), exemplified in the form of electron energy–dependent desorption yields of energetic H^- (1 to 4 eV). These and other fragments emanate from the thin films during electron impact as a result of the formation and subsequent dissociation of electron-molecule resonances RH^{*-}. Each film was ~5 monolayers thick and was prepared and irradiated under UHV conditions (10^{-10} torr). Experimental methods were as described (*14, 22*).



Martin, Burrow, Cai, Cloutier, Hunting & Sanche
PRL (2004)

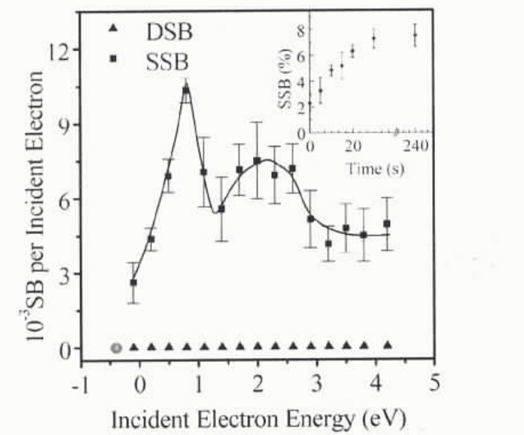


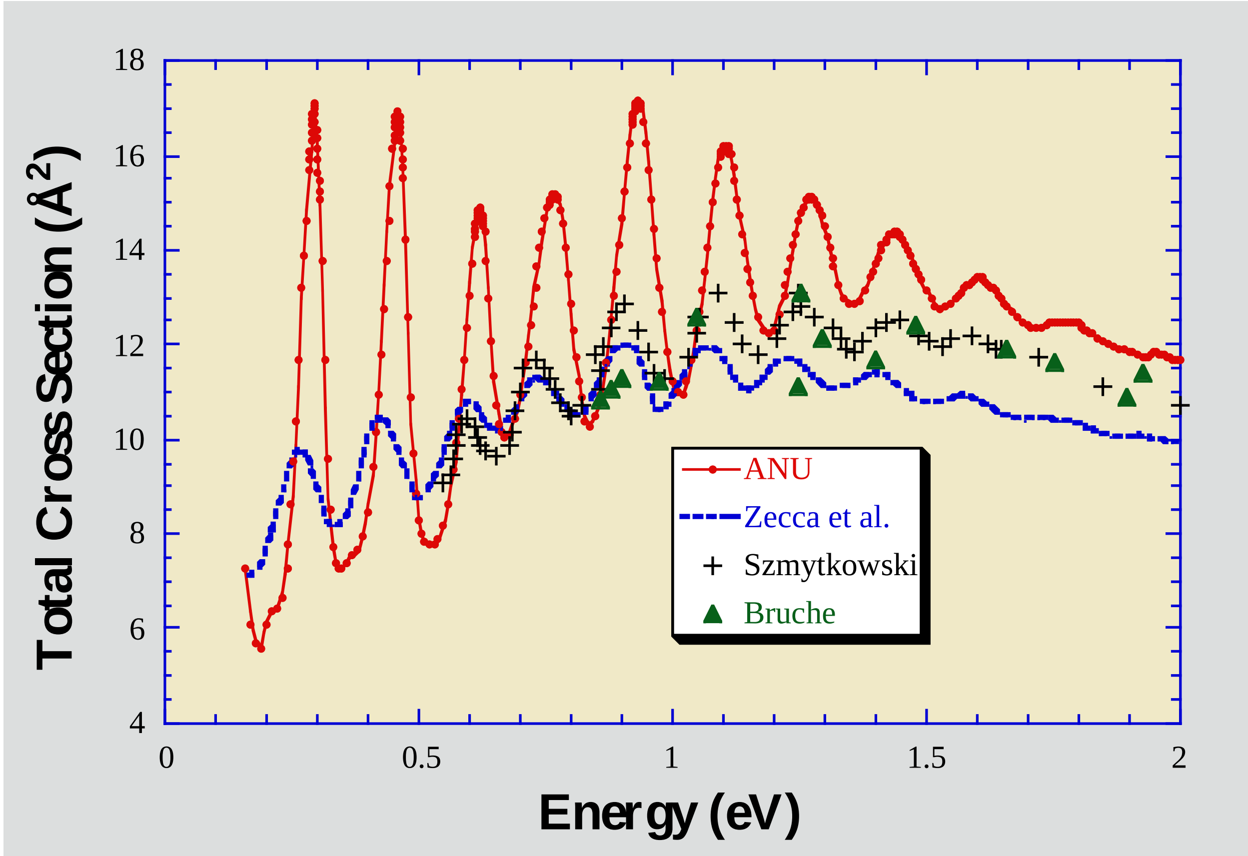
FIG. 1. Quantum yield of DNA single strand breaks (SSBs) and double-strand breaks (DSBs) vs incident electron energy. The inset shows the dependence of the percentage of circular DNA (i.e., SSBs) on irradiation time for 0.6 eV electrons.

068101-2

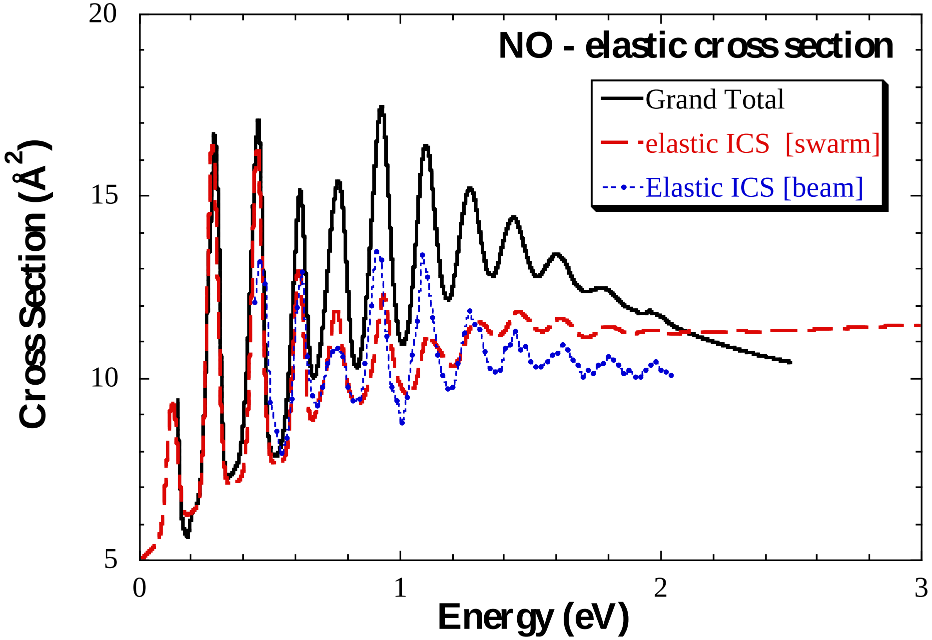
Resonance Excitation in NO Auroral Glow

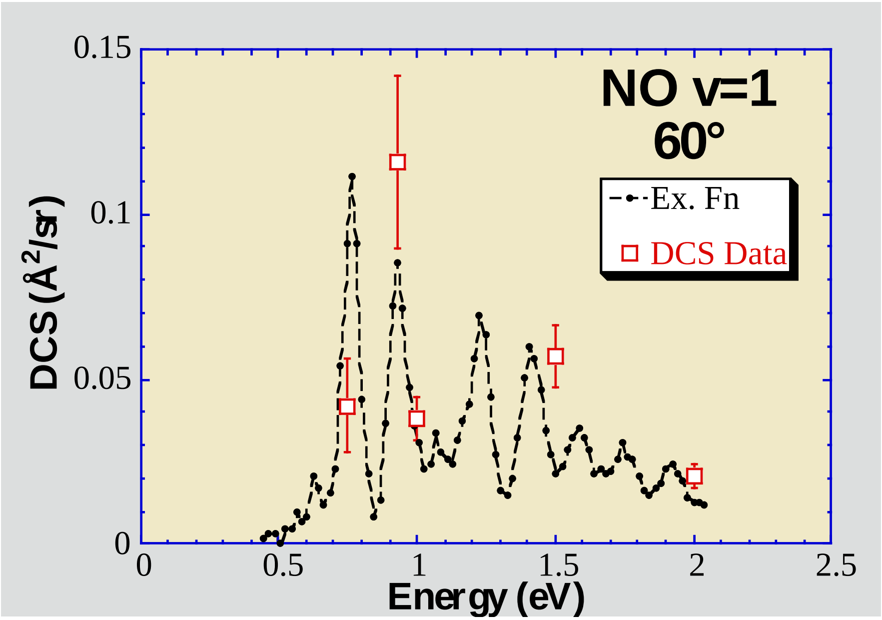
Total Scattering

Nitric Oxide - NO



Elastic and Vibrational - NO





NO - Auroral Emissions

NO is a strong contributor to infrared emissions

– Believed due to **Chemiluminescence**

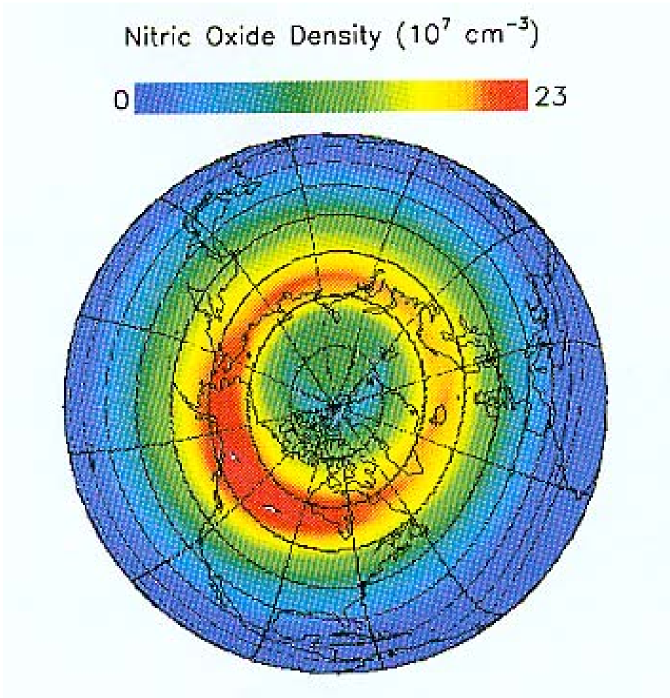
$$N(^2D) + O_2 \Rightarrow NO^*(v = 1-12) + O$$

Auroral Modelling (Cartwright *et al.*)

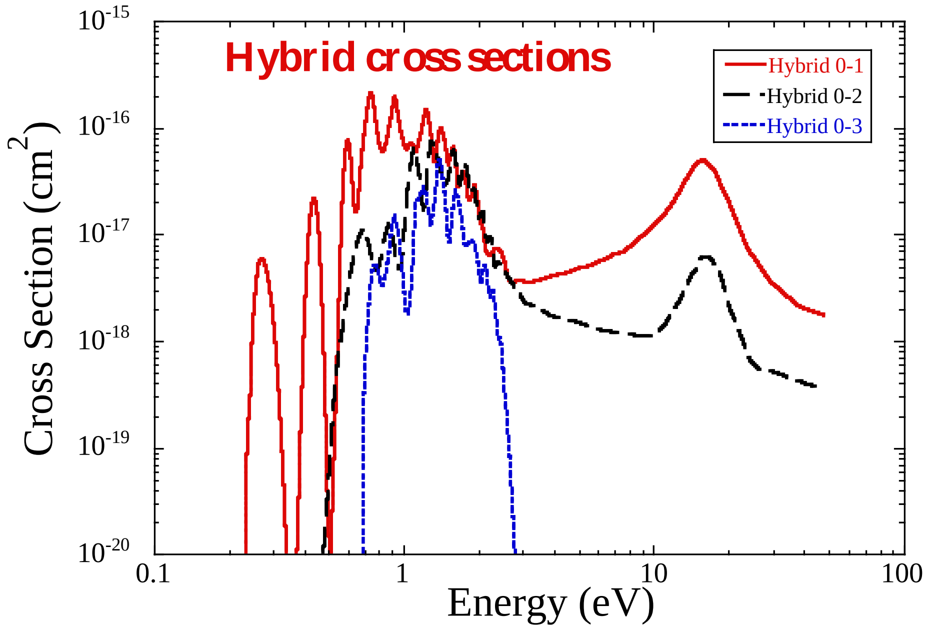
– Predicts
  - NO excited state densities
  - Production of vibrationally excited NO
  - Emission characteristics

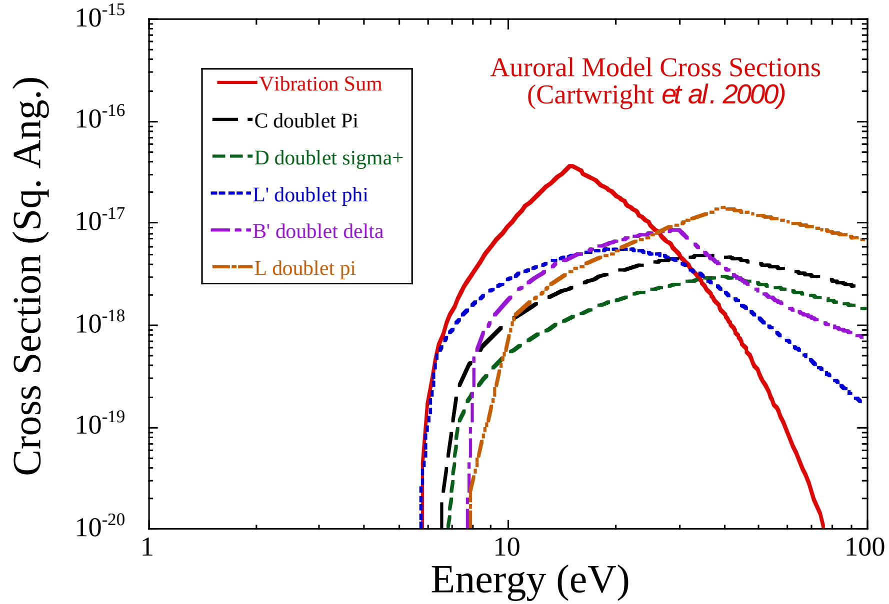
– Assumes no vibrational excitation below 5 eV !!

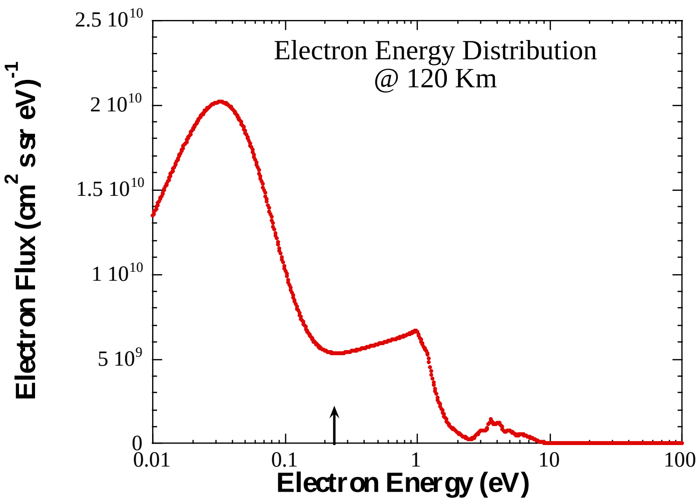
– **Consequences of new measurements?**



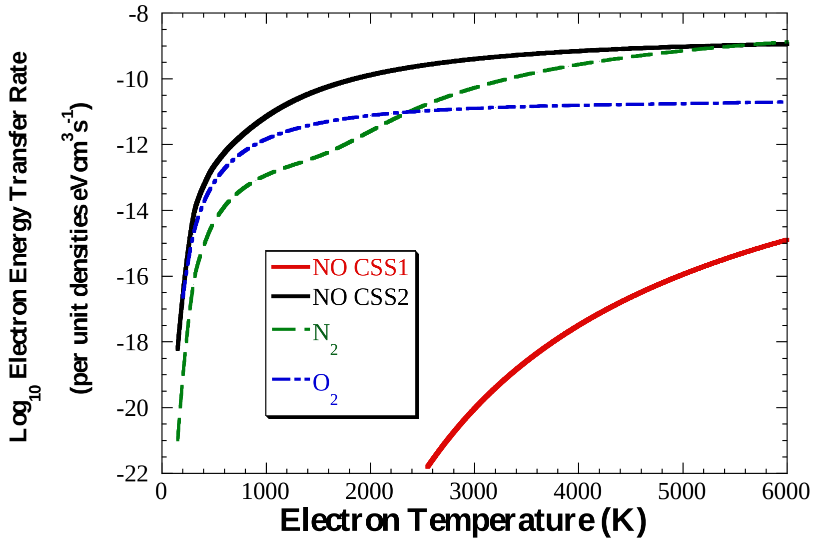
Cross section sets



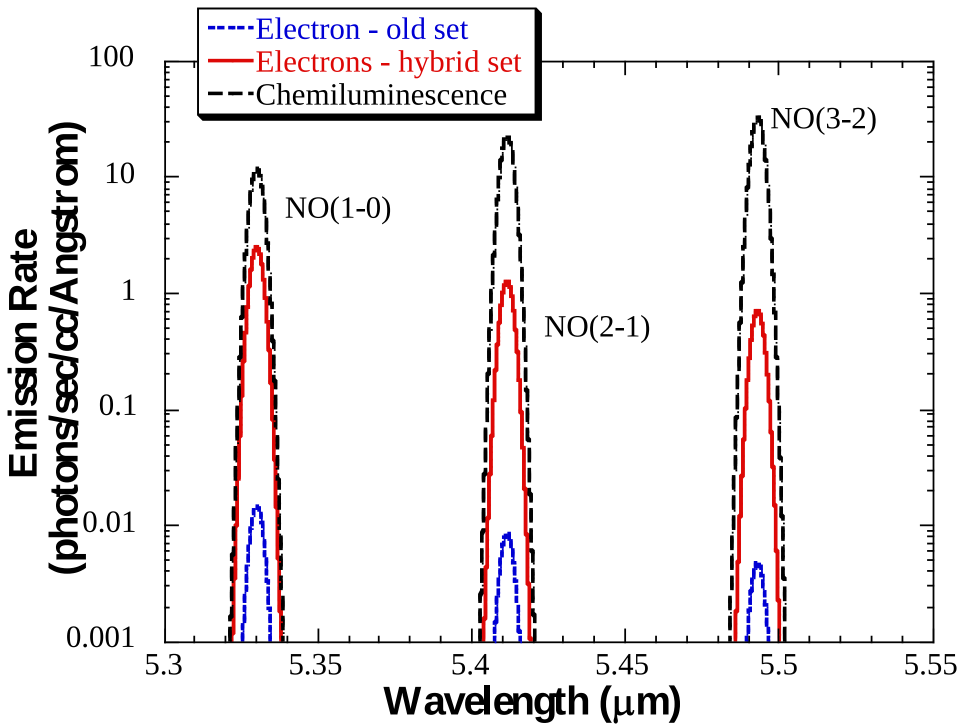




Vibrational Excitation IS important



Data from Rocket-based Measurements



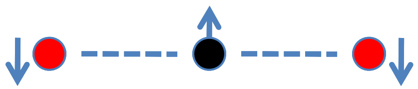
Scattering FROM Excited States

- Low temperature (and other) discharges can contain high equilibrium populations of excited states
- Atoms
  – short and long-lived electronic states
- Molecules
  – short and long-lived electronic states
  – Vibrational excitation
    - e.g. homonuclear diatomic molecules
    - vibrationally excited state decay is optically forbidden
    - large populations can develop

Vibrationally excited CO_2

ground state

First excited state
0.082 eV



Electron scattering from vibrationally excited CO_2 5179

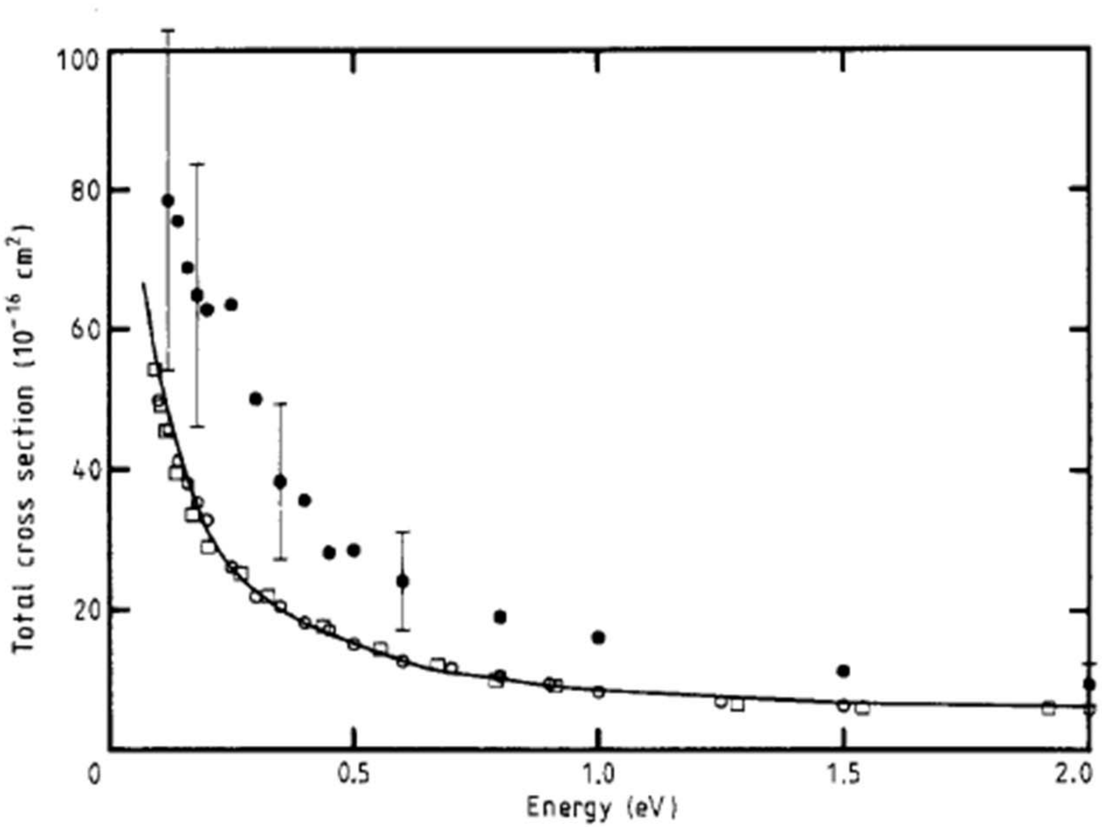


Figure 1. Absolute total cross sections for electron scattering from CO_2 in the energy range 0–2.0 eV. ●, present results for vibrationally excited CO_2: ○, present results for ground-state CO_2; □, Ferch *et al* (1982); ——, theory of Morrison *et al* (1977).

J. Phys B **20** 5175 (1987)

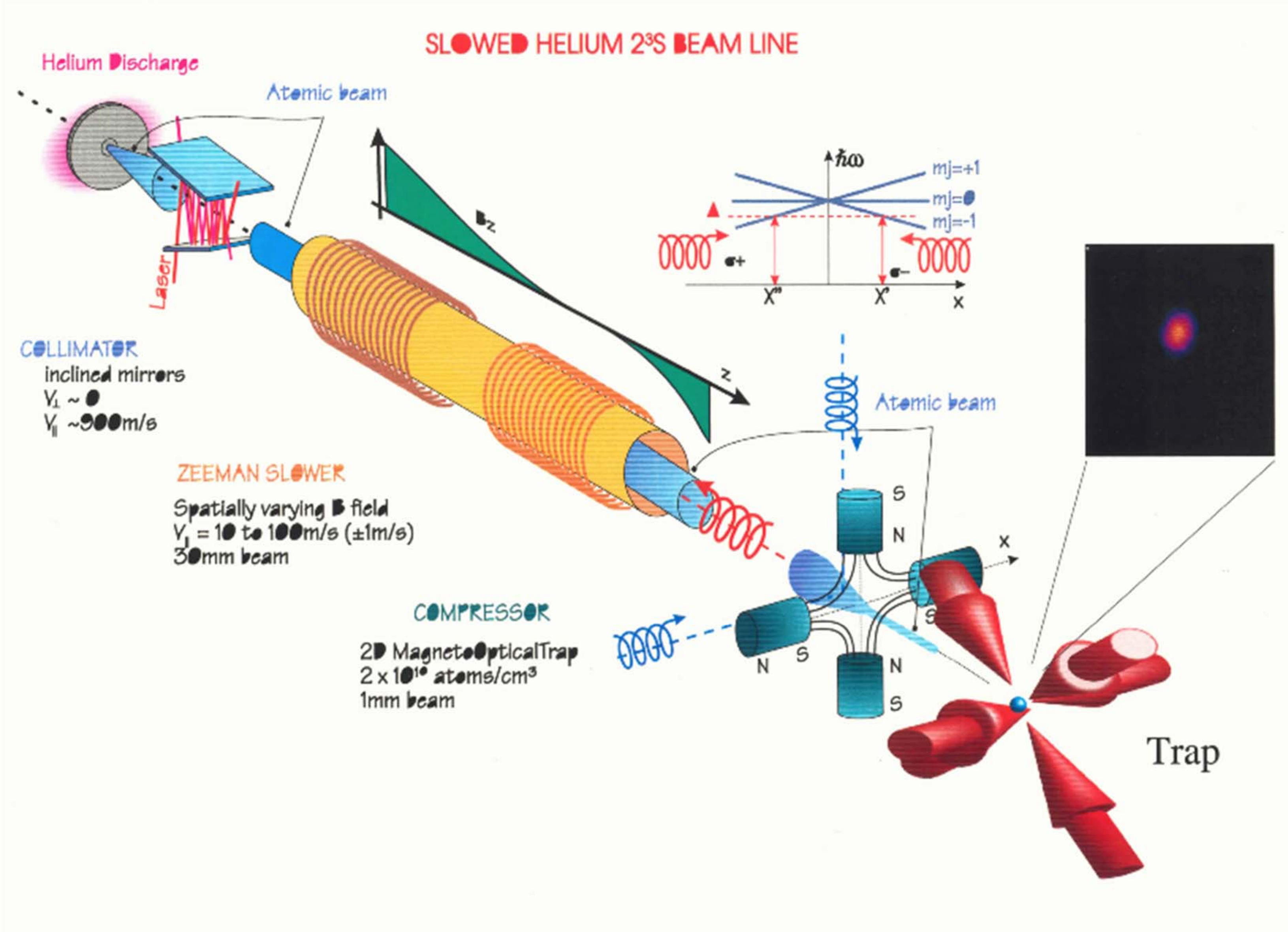
Metastable Excited States

- Metastable atoms and molecules
  - long lifetimes
  - large internal energies
  - low excitation/ionization thresholds
  - HUGE scattering cross sections
  - sources of Penning ionization (e.g. $He^{*}+AB \rightarrow AB^{+} + He + E$)
    - HUGE cross sections (>100 Sq. Ang.)
- Experimental Studies
  - difficult to produce controlled targets
  - low densities
  - easily quenched
  - tough experiments - only a few in literature

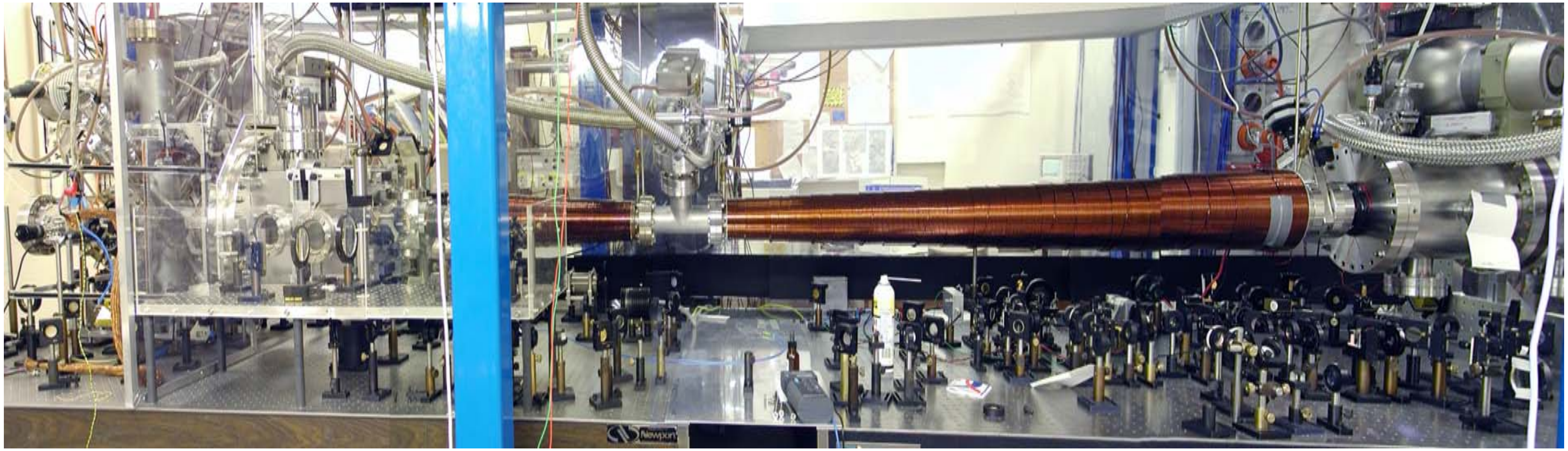
Metastable He (2^3S)

- prototypical system
- long lifetime (~ 8000 secs)
- Loosely bound (4.8 eV)
- highly polarisable (α ~ 150 a.u)
- can ONLY be produced by electron impact
  - discharge-based sources needed
  - low densities (10^7 cm^{-3})
  - large backgrounds (ions, photons, electrons)
- New experiment using laser cooling and trapping techniques

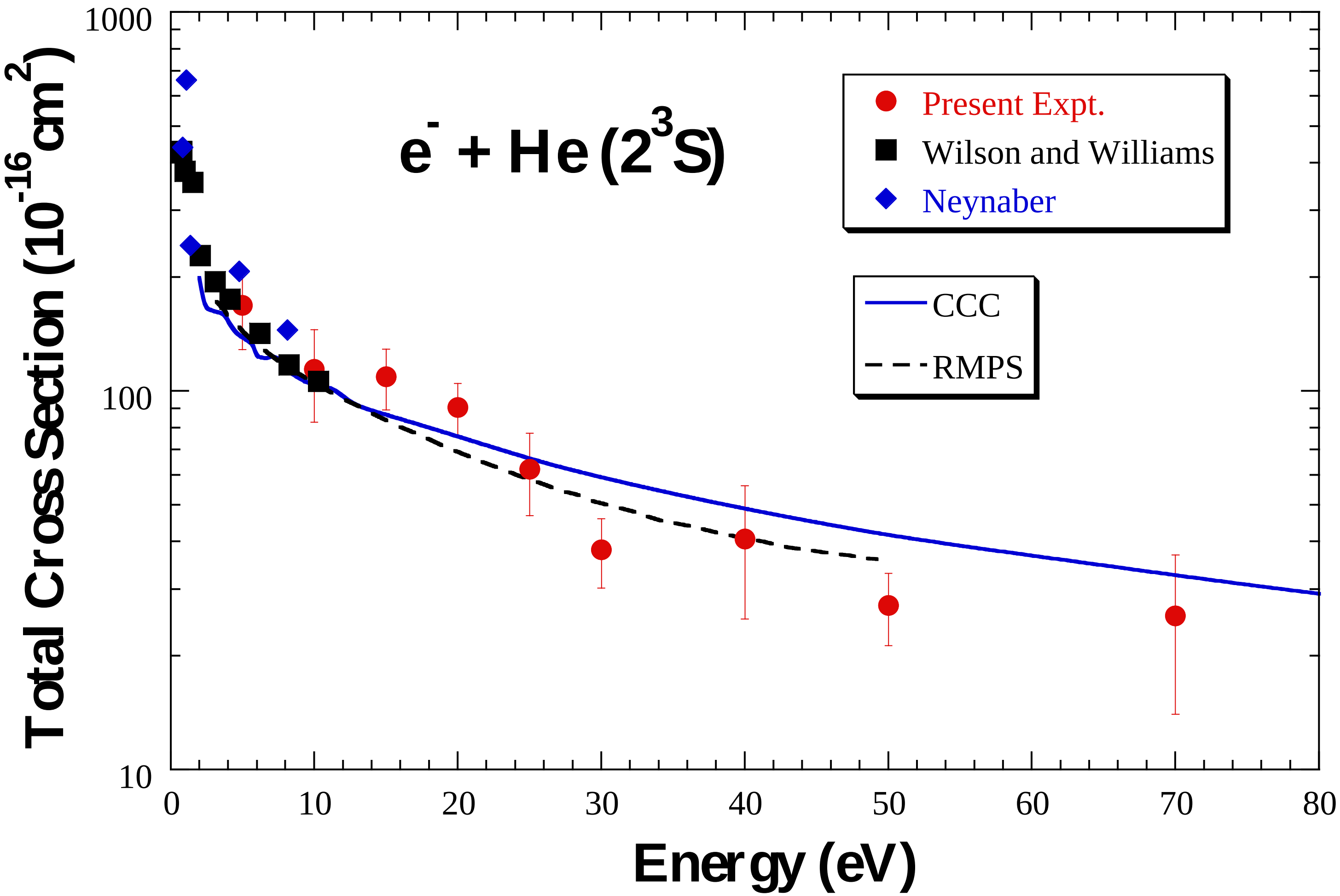
Laser Cooled He* Beam and Trap



Cold He* Beam Apparatus



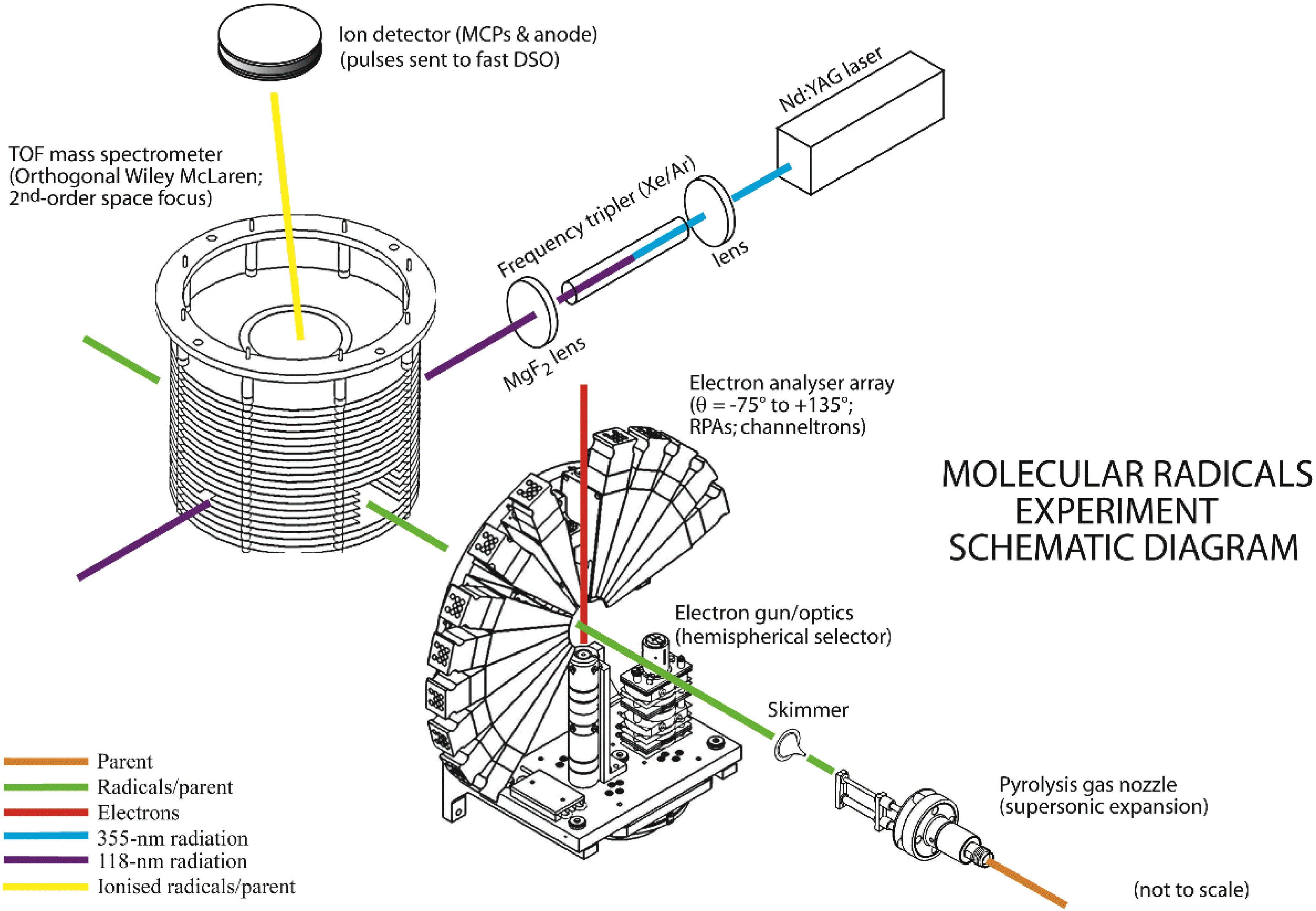
He* Total Cross Section



Uhlmann, Dahl, Truscott, Hoogerland, Baldwin & Buckman PRL **94**, 173201 (2005)

Scattering from Molecular Radicals

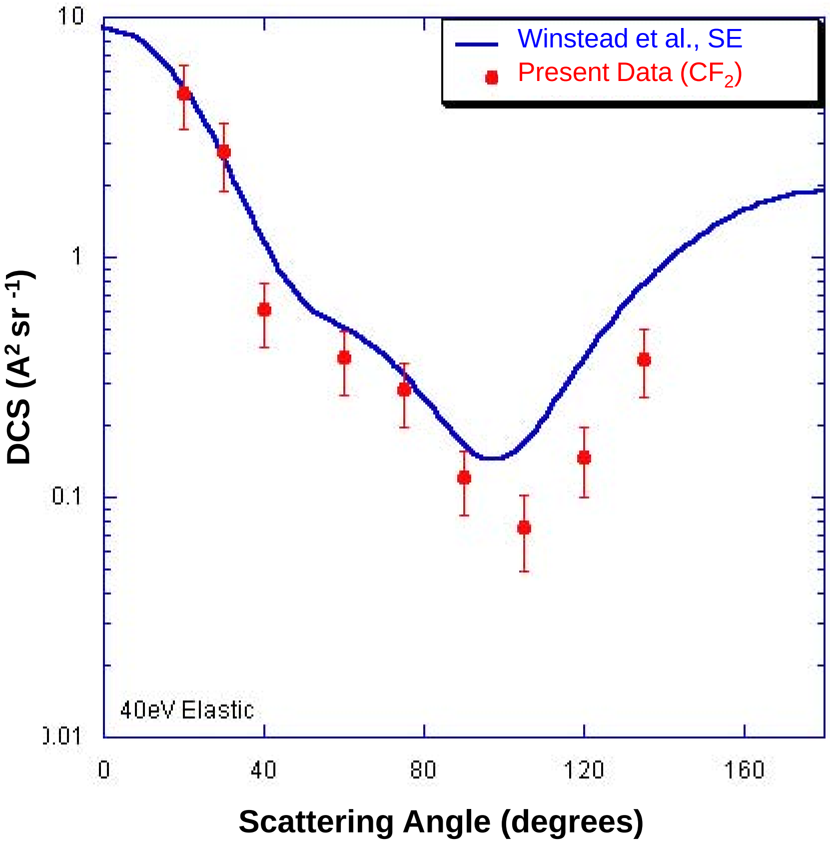
- Radicals readily produced in gas discharges through dissociation
- Electron collision cross sections for highly reactive CF_x (x=1,2,3) radicals are useful for modelling plasmas employed in the semiconductor fabrication industry
- Experimental studies with CF_x ?
  - Rare
  - difficult to produce, characterize, etc….
- Theory?
  - difficult
  - Open shell, highly polarizable, polar, …..
- Present work
  - a new apparatus for measuring absolute elastic cross sections for electron scattering from molecular radicals has been developed
  - results for $e^- + CF_2$ are given to illustrate its potential

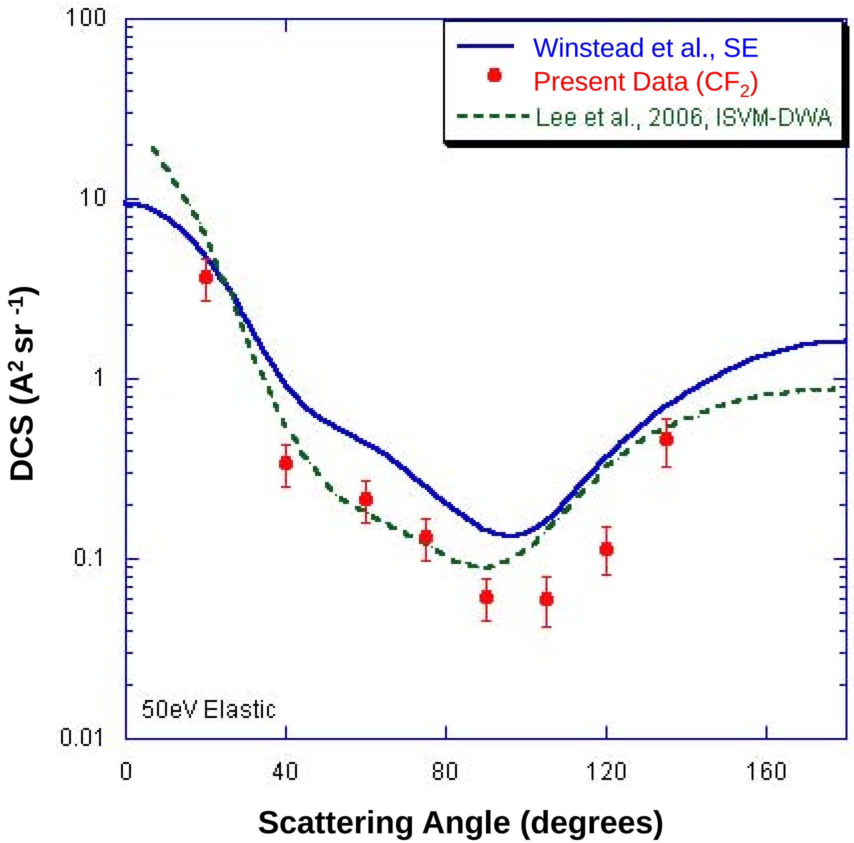


(Maddern *et al. MST*)

Radical Scattering Apparatus

Elastic DCS: CF_2 / CF_4





Some "new" experimental advances

- measurements at all scattering angles
- synchrotron-based electron sources
- trap-based, "magnetised" beams

Some Review Articles

Eur. Phys. J. D (2012) 66: 36
DOI: 10.1140/epjd/e2011-20630-1

THE EUROPEAN PHYSICAL JOURNAL D

Regular Article

Cross section data sets for electron collisions with H_2, O_2, CO, CO_2, N_2O and H_2O

K. Anzai[1], H. Kato[1,a], M. Hoshino[1], H. Tanaka[1], Y. Itikawa[2,b], L. Campbell[3], M.J. Brunger[3,4], S.J. Buckman[5], H. Cho[6], F. Blanco[7], G. Garcia[8], P. Limão-Vieira[1,9], and O. Ingólfsson[10]

Elastic Cross Sections for Electron Collisions with Molecules Relevant to Plasma Processing

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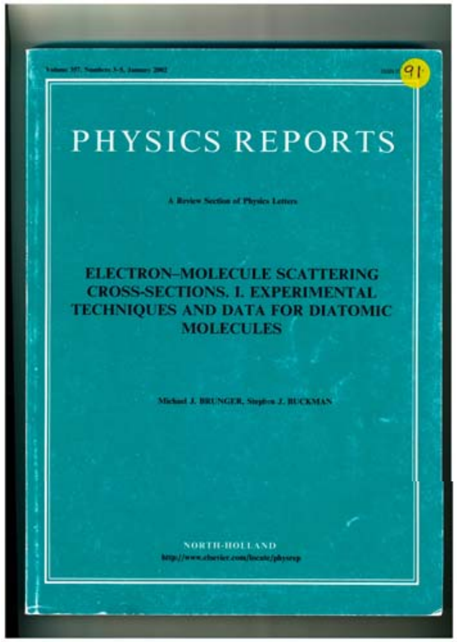
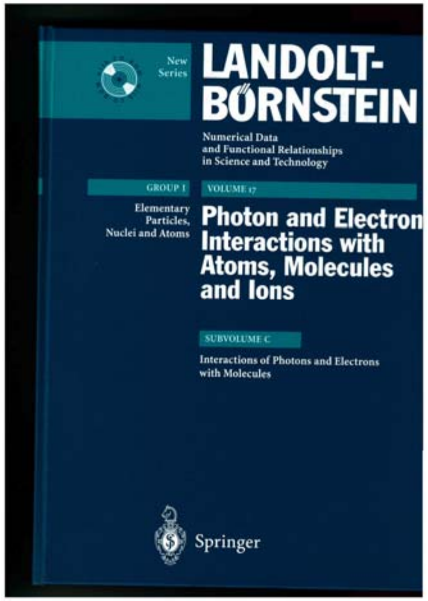
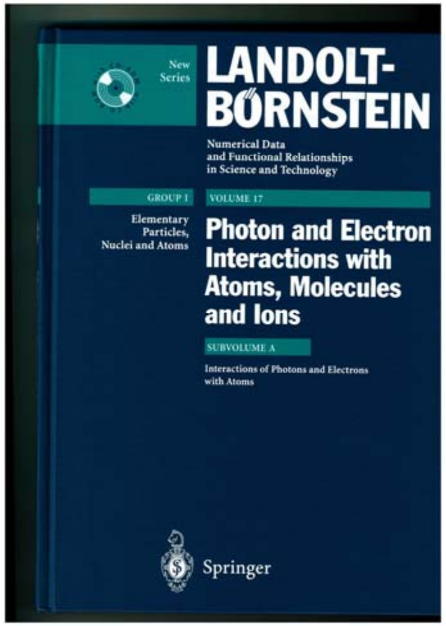
H. Cho[a)]
Physics Department, Chungnam National University, Daejeon 305-764, South Korea

J. Phys. Chem. Ref. Data, Vol. 39, No. 3, 2010

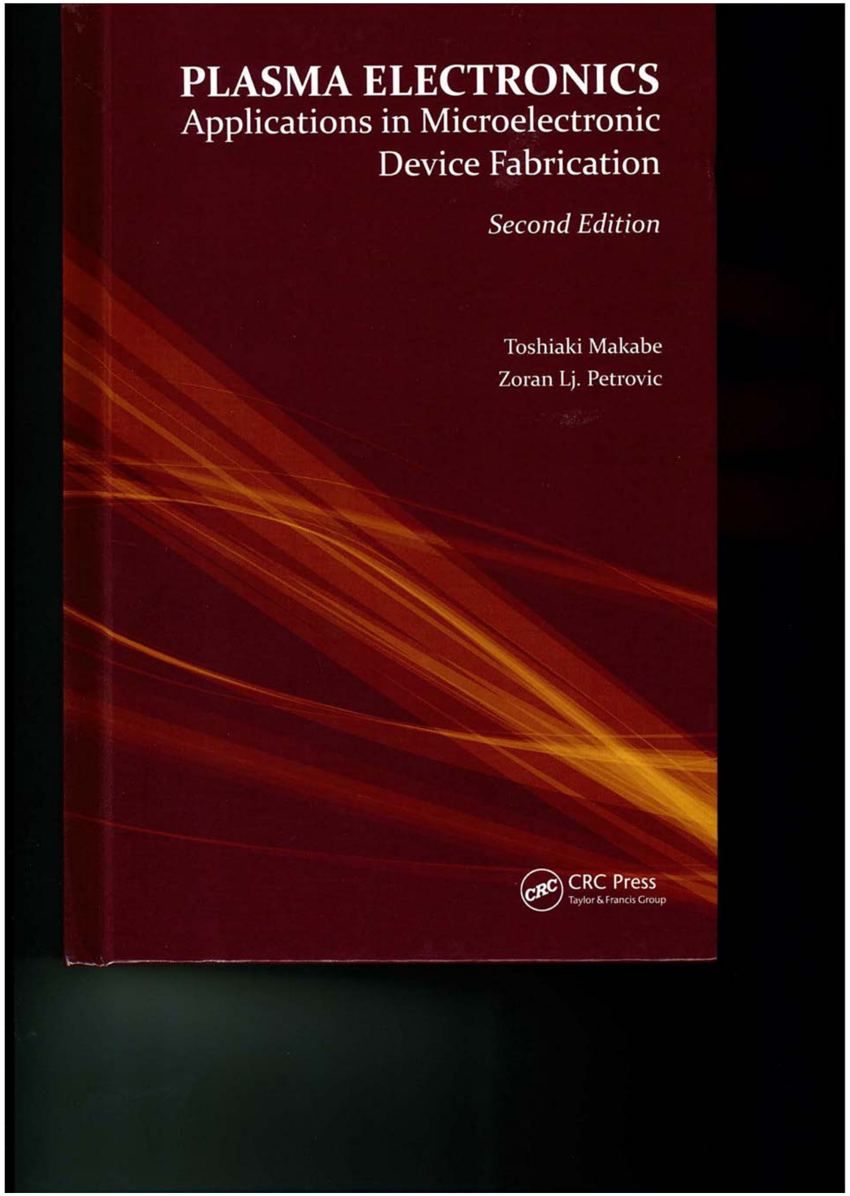






An ideal Text -

Excellent text for connecting cross sections and plasma parameters



Conclusions

- Cross sections ARE important
  - GOOD cross section data is a critical element for a GOOD plasma or discharge model
  - important processes – resonance scattering, excited states, radicals
- How does one judge what is "good"
  - published, peer-reviewed data or calculations
  - reputable laboratories or theoretical groups
  - benchmarked ?
- Don't believe everything you find !
- Be critical and ask questions !
- Databases
  - many now in existence (eg. LXCAT, ...)