Electron transport calculations in detector gas mixtures

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Overview

- Magboltz calculations, recent updates;
- Light emission studies;
- Cluster size and primary clusters (Mip), Fano factors and X-ray cloud size;
- Avalanche simulation;
- Quenching in gas mixtures;
- New argon and xenon level scheme in Magboltz;
- Cluster size calculations of some ILC TPC gases (N_{EPF});
- Plans;
- Request.

} All depends on Penning transfers

Magboltz calculations

- Versions `8.n` now contains some gas files that are fully anisotropic: He, Ne, Ar, Kr, Xe, CO_2, N_2, CH_4 and CF_4.
- This allows them to be used in range, cluster size, Fano program: `http://cern.ch/magboltz`
- Recently extended Ar and Xe database to include ~50 levels.
- Accuracy of argon mixtures with CO_2, N_2 and CH_4 now better than 0.5 %, CF_4: ~1 %

Light emission (primary and avalanches)

- Collaboration with:
  - R. Veenhof, CERN
  - C. de Oliveira, Aveiro
  - J. Veloso, Aveiro
  - A. Ferreira, Aveiro
  - J. dos Santos, Coimbra
  - C. Monteiro, Coimbra
- Physics of light emission
  - Understanding of pure gases;
  - Pressure dependence ⇒
  - Quenching in gas mixtures by Penning transfer

Pure gases

- Radiation trapping of resonance levels
  - Resonance levels are those that are connected to the ground state by dipole-allowed transitions.
  - Resonance level decay → immediate reabsorption by ground state atoms.
  - Typical absorption X-section ~200 Mbarn at atmospheric pressure, 1 μm absorption distance.
  - Escape route for trapped radiation by excimer formation: $Ar^* + Ar \rightarrow Ar_2^*$
  - Excimer radiation is not trapped at atmospheric pressure, very few ground state dimers exist.

Radiation trapping (cont'd)

- Radiation trapping in molecular gases is much reduced:
  $\lambda_{abs} = N_{EPF}\,\sigma_{abs}, \quad N_{EPF} \neq N_{atmos}$
- Emission and absorption now spread over vibrational and rotational levels of molecular states:
  λ can now be ~100 μm.

Pressure dependence

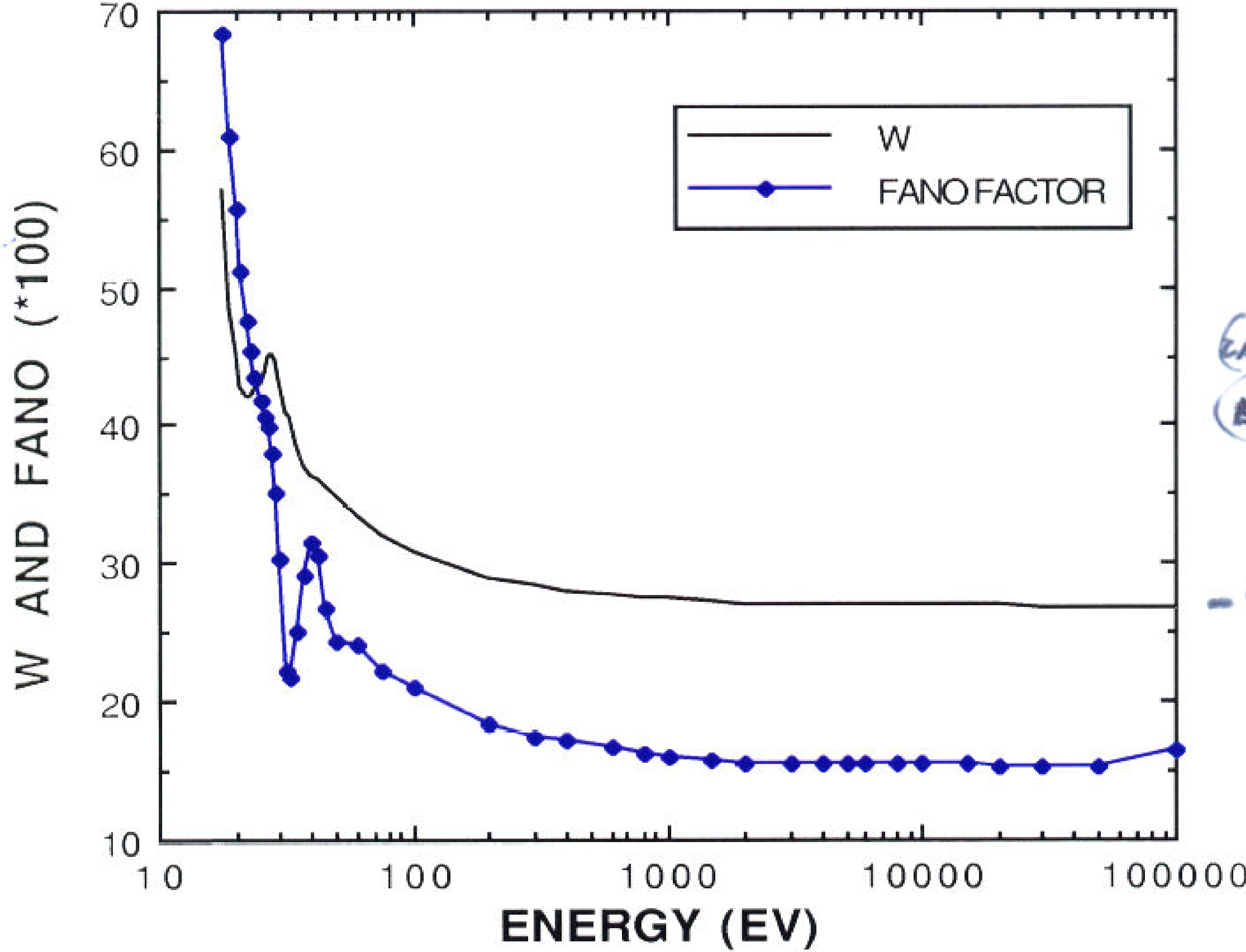
- Collisional mixing: 760 Torr – 1 ns collision time.
- Mixing will alter the calculated level populations probably in the direction of a more statistical distribution ($2J+1$).
- 2nd program to follow cascade decay of excited states
  - at 760 Torr good approximation
    each excited state → 1 excimer decay;
  - below 10 Torr
    resonance trapping and collisional mixing reduced;
  - below 10^{-2} Torr
    resonance trapping fails and fewer excimers produced.

Cluster size, primary clusters, Fano factors, X-ray cloud size

- MIP cluster size:
  - Penning transfer within each cloud increases cluster size.
- Primary clusters:
  - 1 electron clusters are produced by primary excitation.
- X-ray Fano factors:
  - increase in electron number per X-ray by Penning.
- X-ray cloud size:
  - Range now given correctly by completely anisotropic X-sections.

- All the above observables can be calculated in electric and magnetic fields by program MIP on the website.
- Program allows positiion of each electron to be output. This option can be used to develop software algorithms to improve resolution.

FANO FACTOR AND EV/ION PAIR IN ARGON



(CALC) $F_1 \approx 0.17$

(EXP) $F_1 = 0.18(1)$

— W = 26.8 eV = F_0

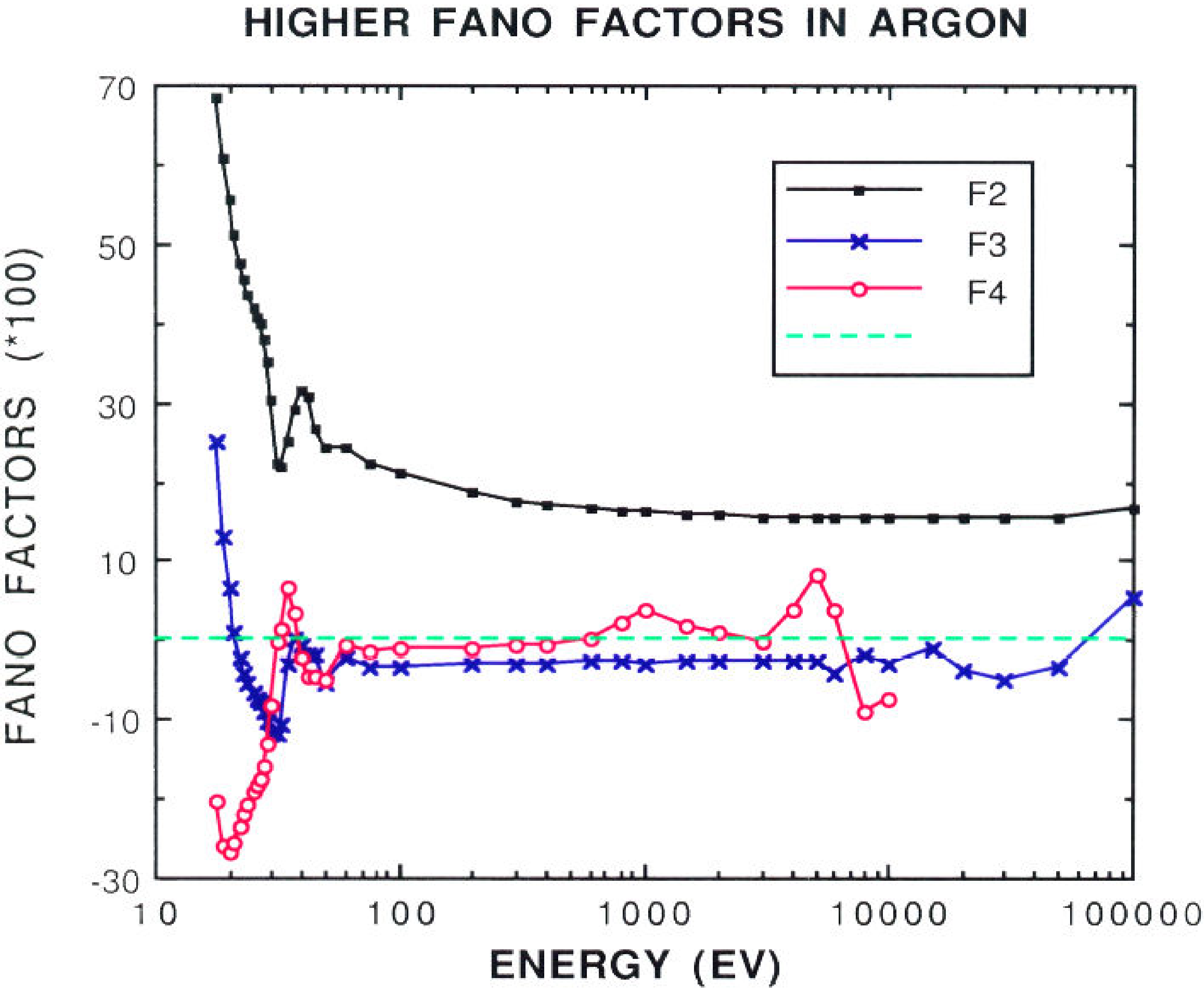
W_{exp} = 26.4 eV.

$AR^* + AR \rightarrow AR_2^+ + e^-$

~ 1–2%

AT

760 TORR


HIGHER FANO FACTORS IN ARGON
FANO FACTORS (*100)
70
50
30
10
-10
-30
10
100
1000
10000
100000
ENERGY (EV)
F2
F3
F4

Avalanche simulation

- When Penning transfers are better understood, develop software of avalanche fluctuations in a “flat field”.

- Useful for Micromegas simulation.

Quenching in gas mixtures

- In gas mixtures, radiation trapping no longer exists. Resonance level decays can now be absorbed by the molecular component to give breakup or photoionisation of the quencher molecule.
- The ratio of the photoionisation to photoabsorption X-section is sometimes called the photoionisation or quantum efficiency. See Berkowitz. Typically:

- For energies > 5 eV above the moleculat ionisation threshold, quantum efficiency = 100 %.

Argon and xenon levels

- Ar and Xe levels now expanded to 50 levels in Magboltz. Included are all dipole transition strengths in xenon. Used "BEF" scaling:

$$\sigma(E) = \frac{E}{E + B + E_{exc}} \sigma_{Born}(E)$$

B = binding energy

E_{exc} = transition energy

Kim, Phys. Rev. A 64 (2001) 032713

Kim and Stone, Phys. Rev. A 64 (2001) 052707

Kim and Descaux, Phys Rev A 66 (2002) 012708

- Previously used low energy modifiers:

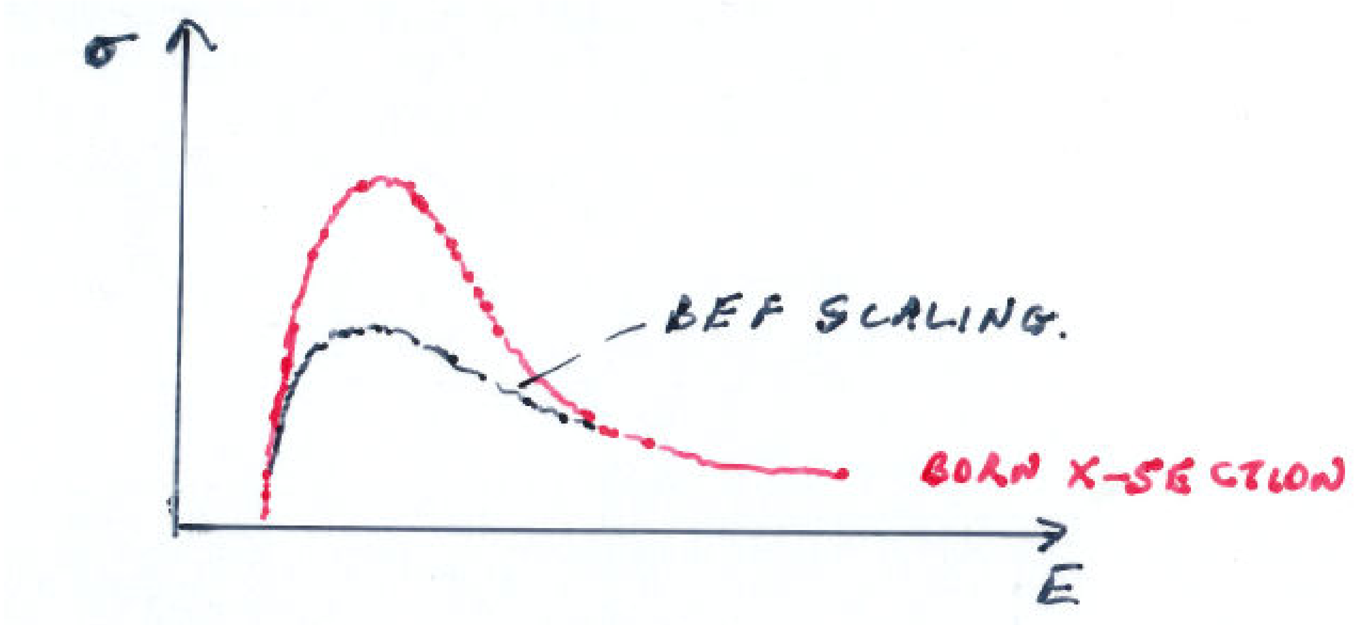
$$\sigma(E) = \left[1 - \left(E_{ex} / mc^2\beta^2\right)^{\alpha}\right]^{\beta} / \left(mc^2\beta^2\right)^{\gamma}$$

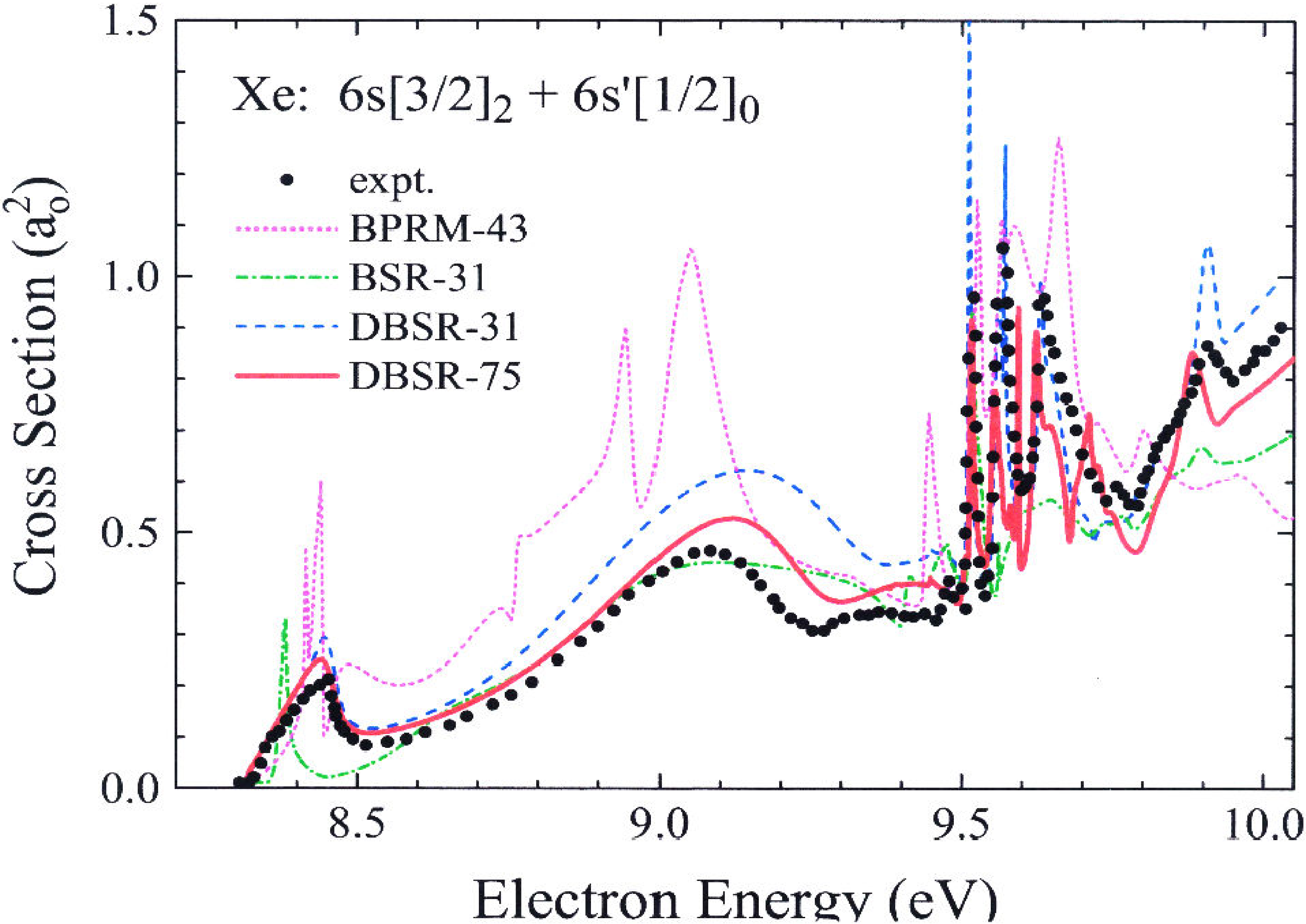
Bretagne et al., J. Phys. D 19 (1986) 761.

- "BEF" scaling gives better agreement with experimental data.

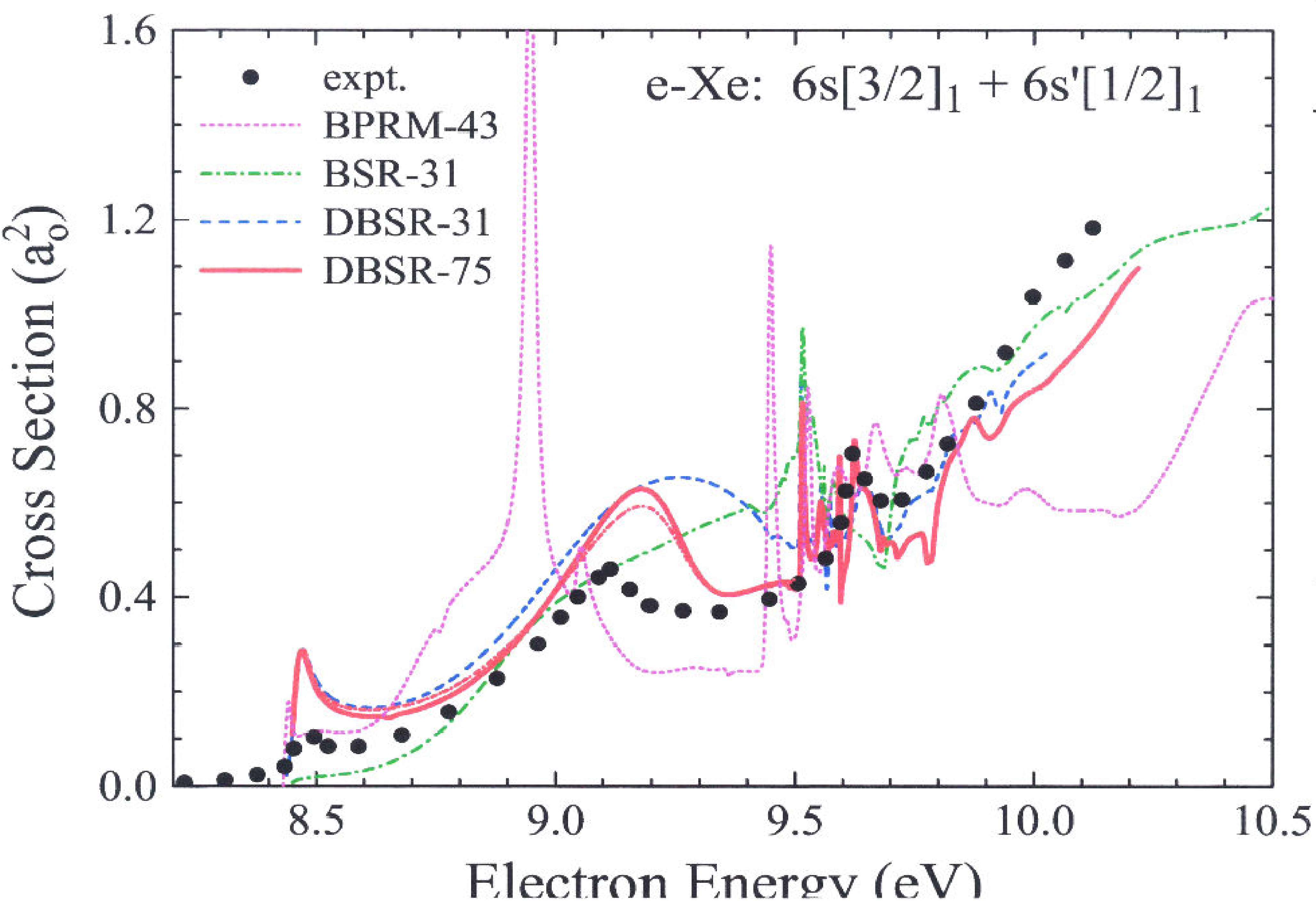
Resonance region

- The resonance region close to threshold is given by Dirac fully relativistic calculations by K. Bartschat.
- X-sections for argon and xenon include X-sections from p-states given by light emission in ~1 mTorr by the Wisconsin group of Fons, Boffard and Lin.





Xe: 6s[3/2]2 + 6s'[1/2]0
expt.
BPRM-43
BSR-31
DBSR-31
DBSR-75
Cross Section (a_o^2)
Electron Energy (eV)
1.5
1.0
0.5
0.0
8.5
9.0
9.5
10.0



e-Xe: 6s[3/2]1 + 6s'[1/2]1
expt.
BPRM-43
BSR-31
DBSR-31
DBSR-75
Cross Section (a0^2)
Electron Energy (eV)
0.0
0.4
0.8
1.2
1.6
8.5
9.0
9.5
10.0
10.5

Calculations for some ILC TPC gases

He/CO_2 70/30

No Penning:
$N_i = 12.41$

Penning
$N_i = 13.45$

Cluster size	No Penning [%]	Incl. Penning [%]
1	75.4	75.3
2	13.1	12.9
3	4.2	4.3
4	2.0	2.0
5	1.14	1.18
6	0.73	0.71
7	0.52	0.53
8	0.39	0.38
9	0.30	0.30
10	0.24	0.24
11	0.20	
12	0.16	
13	0.13	
14	0.12	
15	0.094	
16	0.091	
17	0.075	
18	0.072	
19	0.059	
20	0.054	
>20	0.96	

Fe55 X-Rays:

No Penning
$N_e = 171$
$F = 0.275$

Penning
$N_e = 186$
$F = 0.228$

Calculations for some ILC TPC gases

$Ar/CF_4/C_4H_{10}$ 95/3/2

1% cluster absorption

No Penning:
$N_i = 25.35$

Penning (20%)
$N_i = 25.25$

Cluster size	No Penning [%]	Incl. Penning [%]
1	64.7	61.2
2	17.6	19.3
3	6.3	6.9
4	3.1	3.4
5	1.8	2.0
6	1.2	1.3
7	0.83	0.91
8	0.61	0.67
9	0.47	0.52
10	0.37	0.40
11	0.30	0.32
12	0.25	0.28
13	0.20	0.23
14	0.18	0.19
15	0.16	0.17
16	0.13	0.15
17	0.12	0.13
18	0.10	0.12
19	0.092	0.10
20	0.087	0.091
>20	1.5	1.6

Fe55 X-Rays:

No Penning
$N_e = 225$
$F = 0.153$

Penning
$N_e = 242$
$F = 0.151$

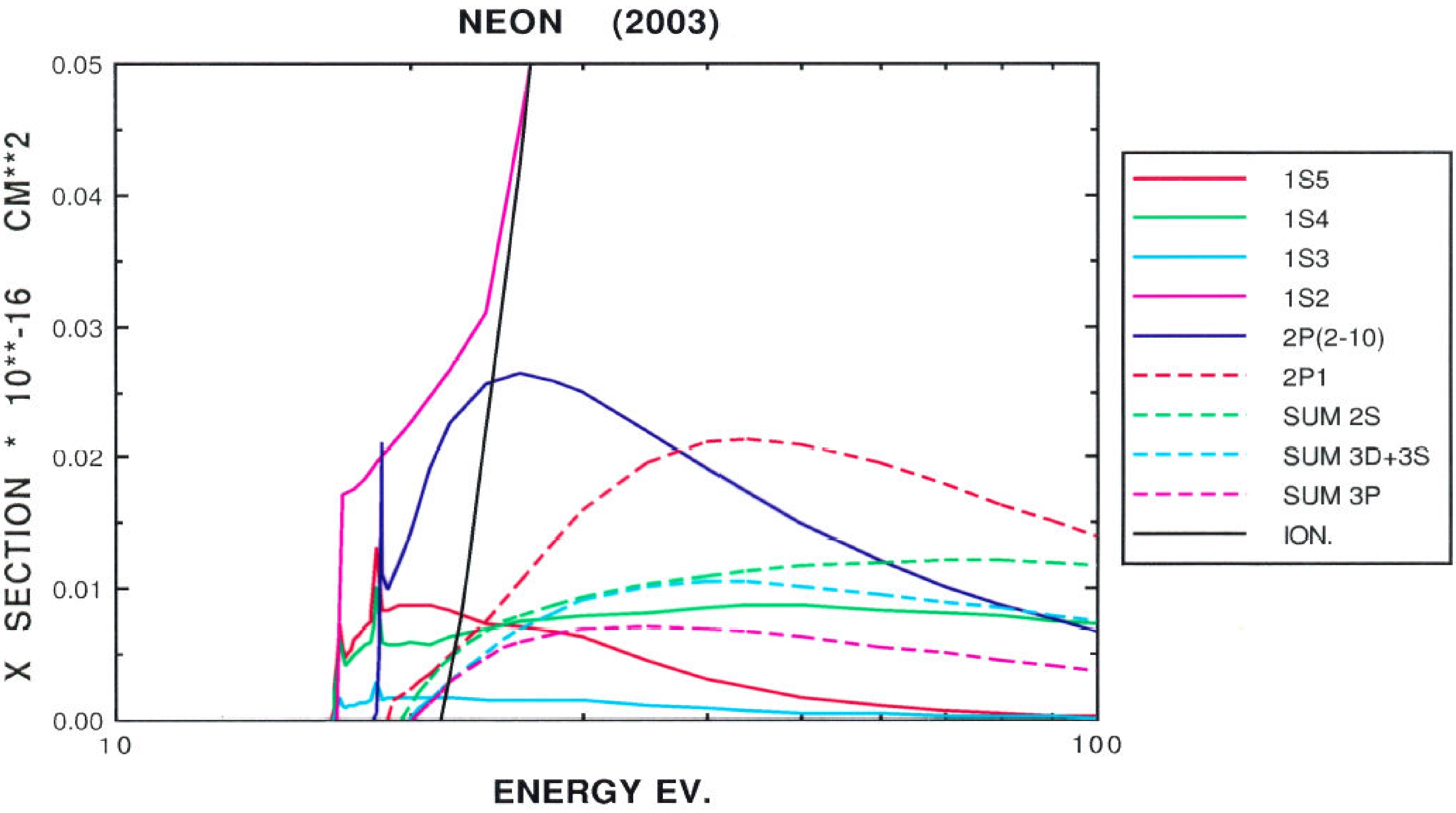
Plans – no priorities yet

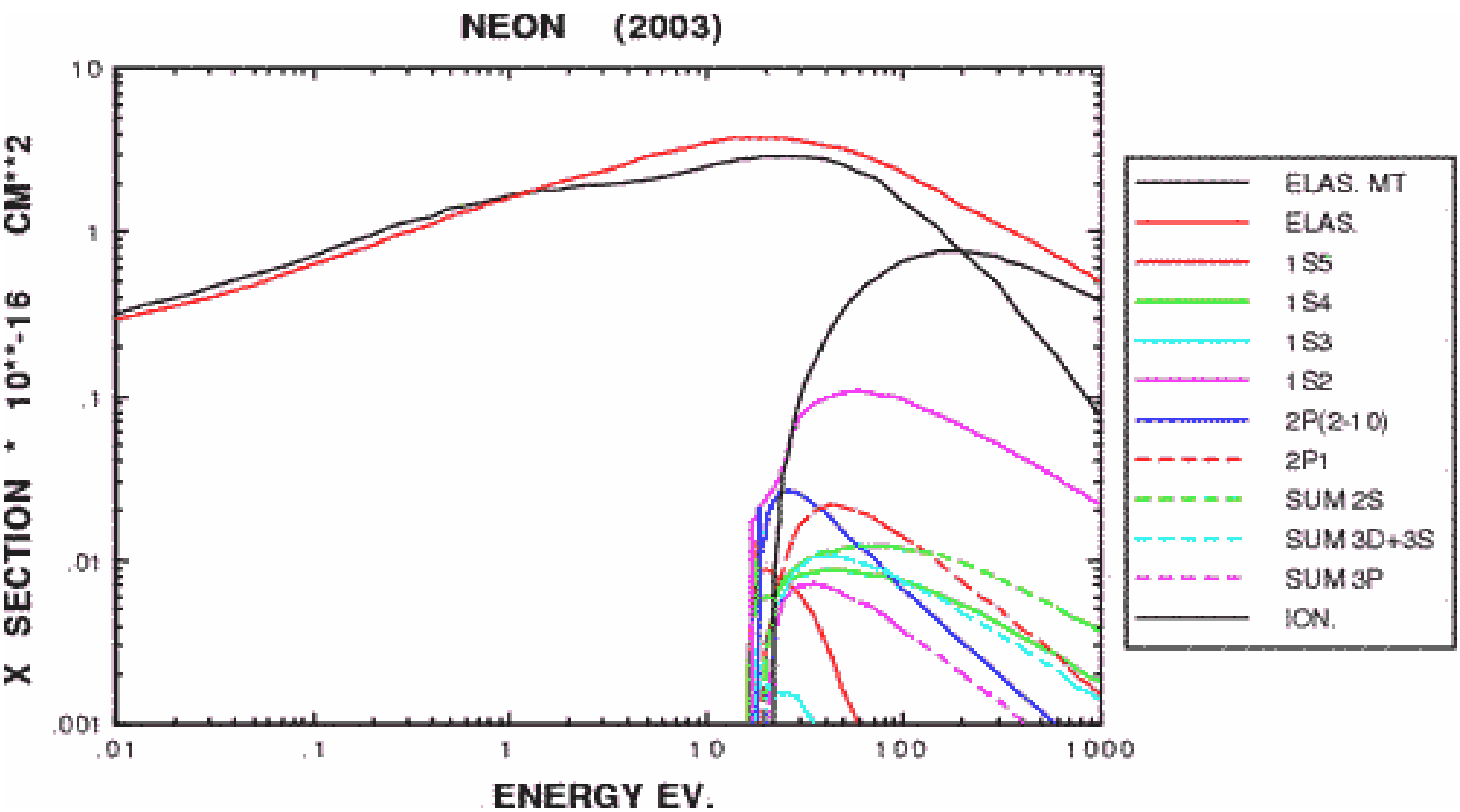
- Upgrade MIP program to calculate:
  - fluctuations in light emission,
  - Fano factors of light emission assuming all excited states are converted to excimers.
- Repeat upgrades to full anisotropy for helium and hydrogen with more extensive excitation level schemes.
- Upgrade $C_2H_4F_2$, RPC request.
- Introduce phonon scattering model for liquids.

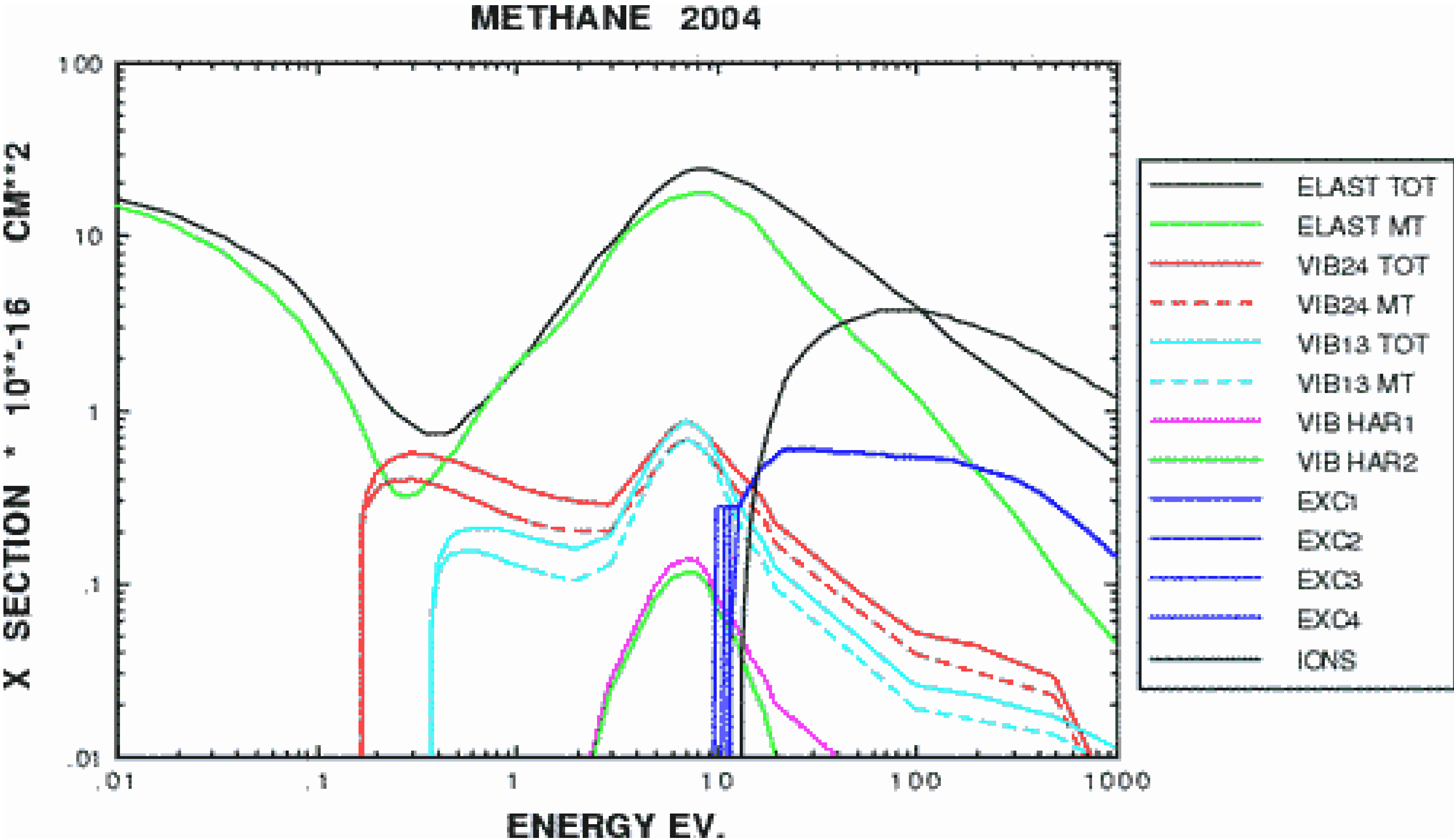
And a request ...

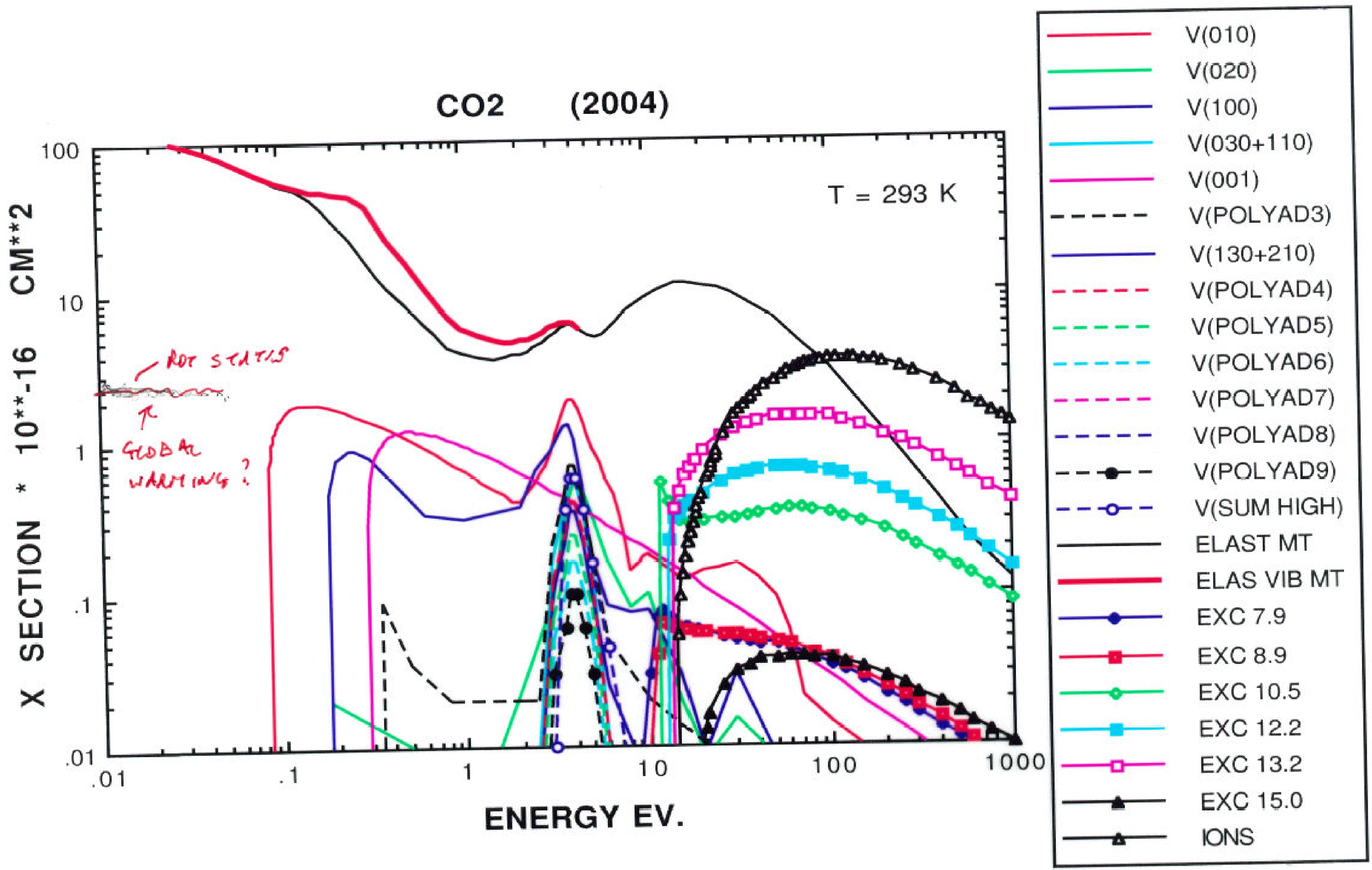
- Finally, a request for someone to repeat the measurement of F. Rieke and W. Prepejchal with modern electronics. [Phys. Rev. A **6** (**1972**) **1**507-1519]

- This is one of the most important papers in atomic physics as well as having great importance for understanding chamber performance.

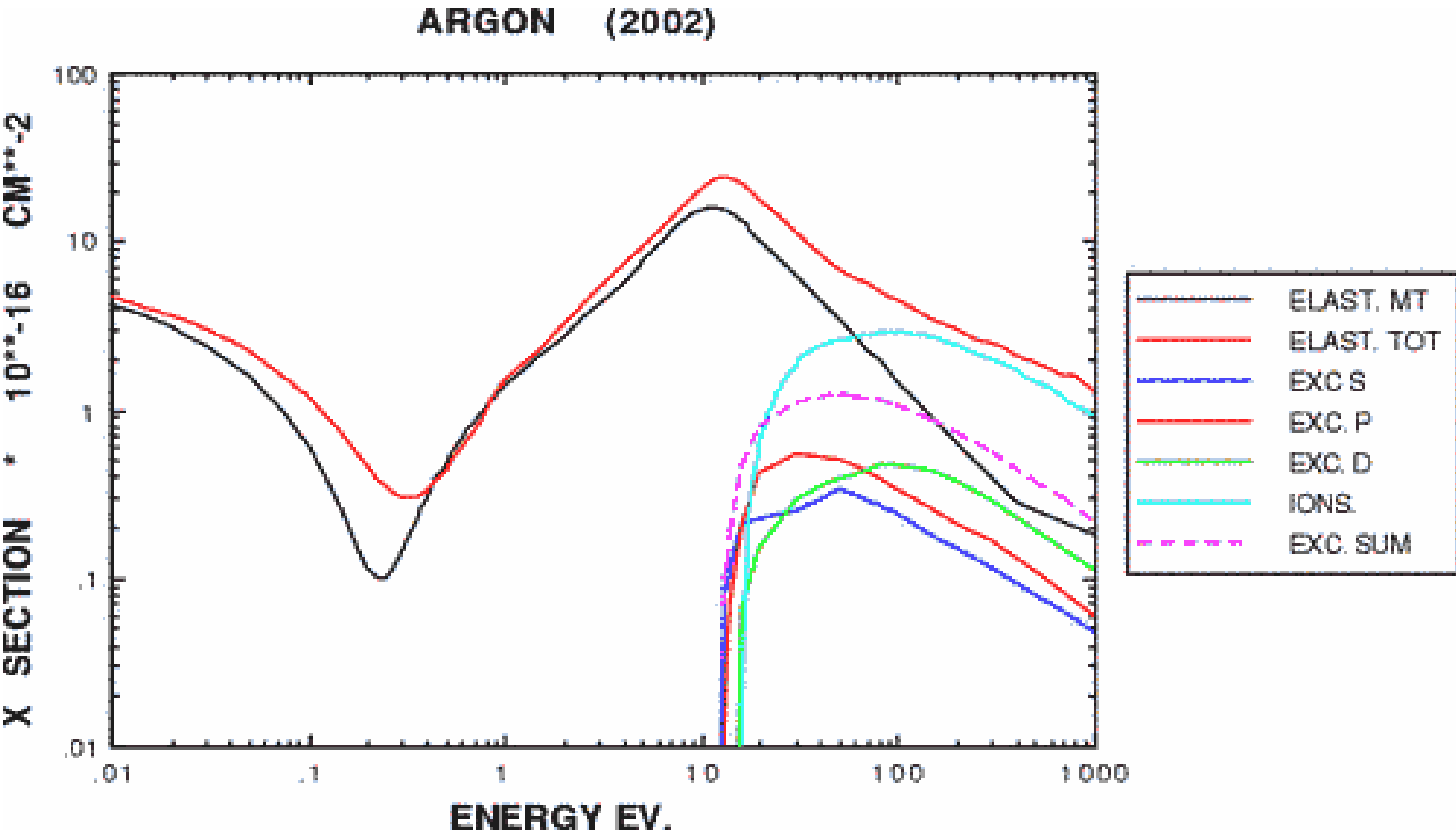

NEON (2003)
X SECTION * 10**-16 CM**2
0.05
0.04
0.03
0.02
0.01
0.00
10
100
ENERGY EV.
1S5
1S4
1S3
1S2
2P(2-10)
2P1
SUM 2S
SUM 3D+3S
SUM 3P
ION.

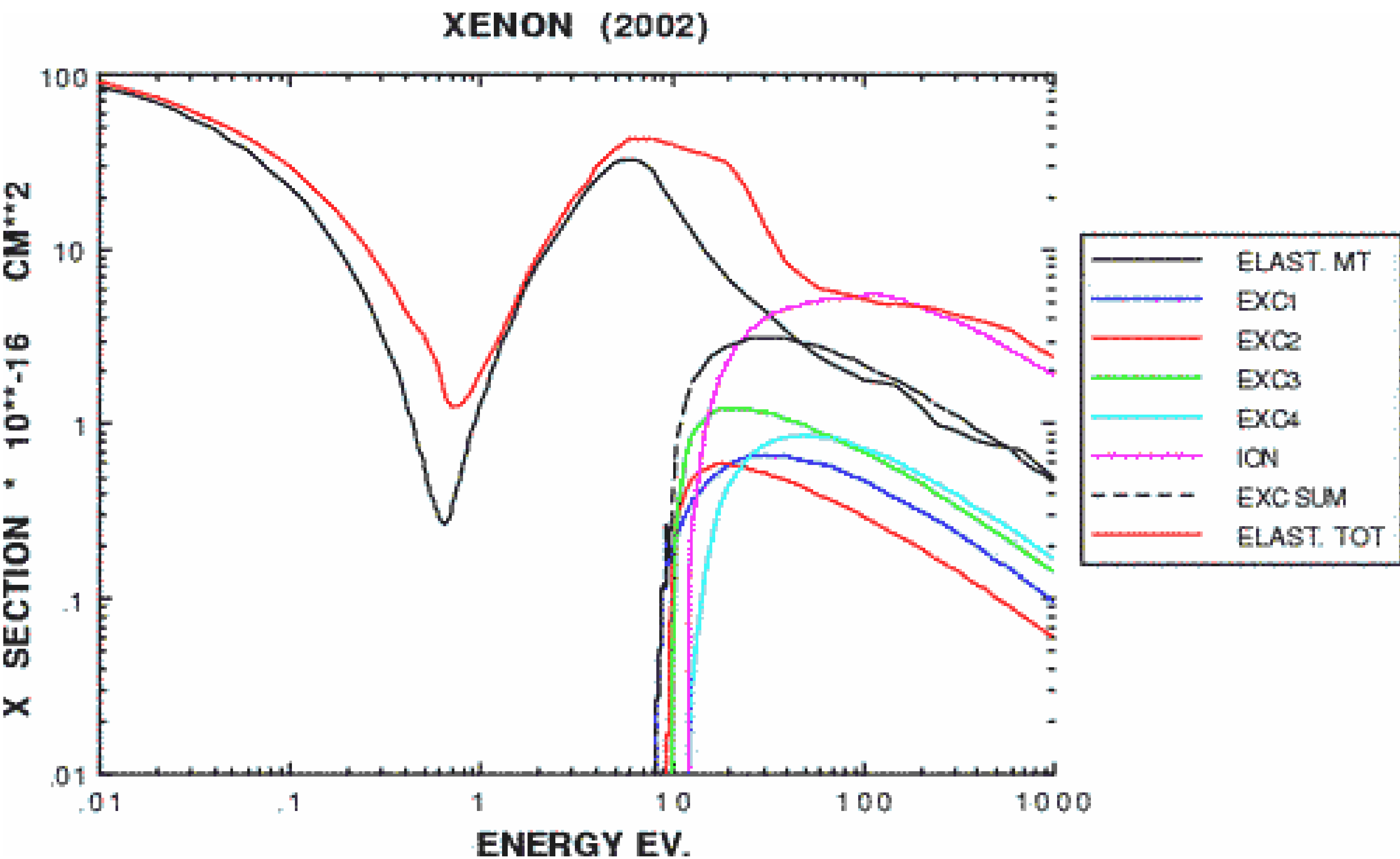

NEON (2003)
X SECTION * 10**-16 CM**2
ENERGY EV.
10
1
.1
.01
.001
.01
.1
1
10
100
1000
ELAS. MT
ELAS.
1S5
1S4
1S3
1S2
2P(2-10)
2P1
SUM 2S
SUM 3D+3S
SUM 3P
ION.


METHANE 2004
X SECTION * 10**-16 CM**2
100
10
1
.1
.01
.01
.1
1
10
100
1000
ENERGY EV.
ELAST TOT
ELAST MT
VIB24 TOT
VIB24 MT
VIB13 TOT
VIB13 MT
VIB HAR1
VIB HAR2
EXC1
EXC2
EXC3
EXC4
IONS

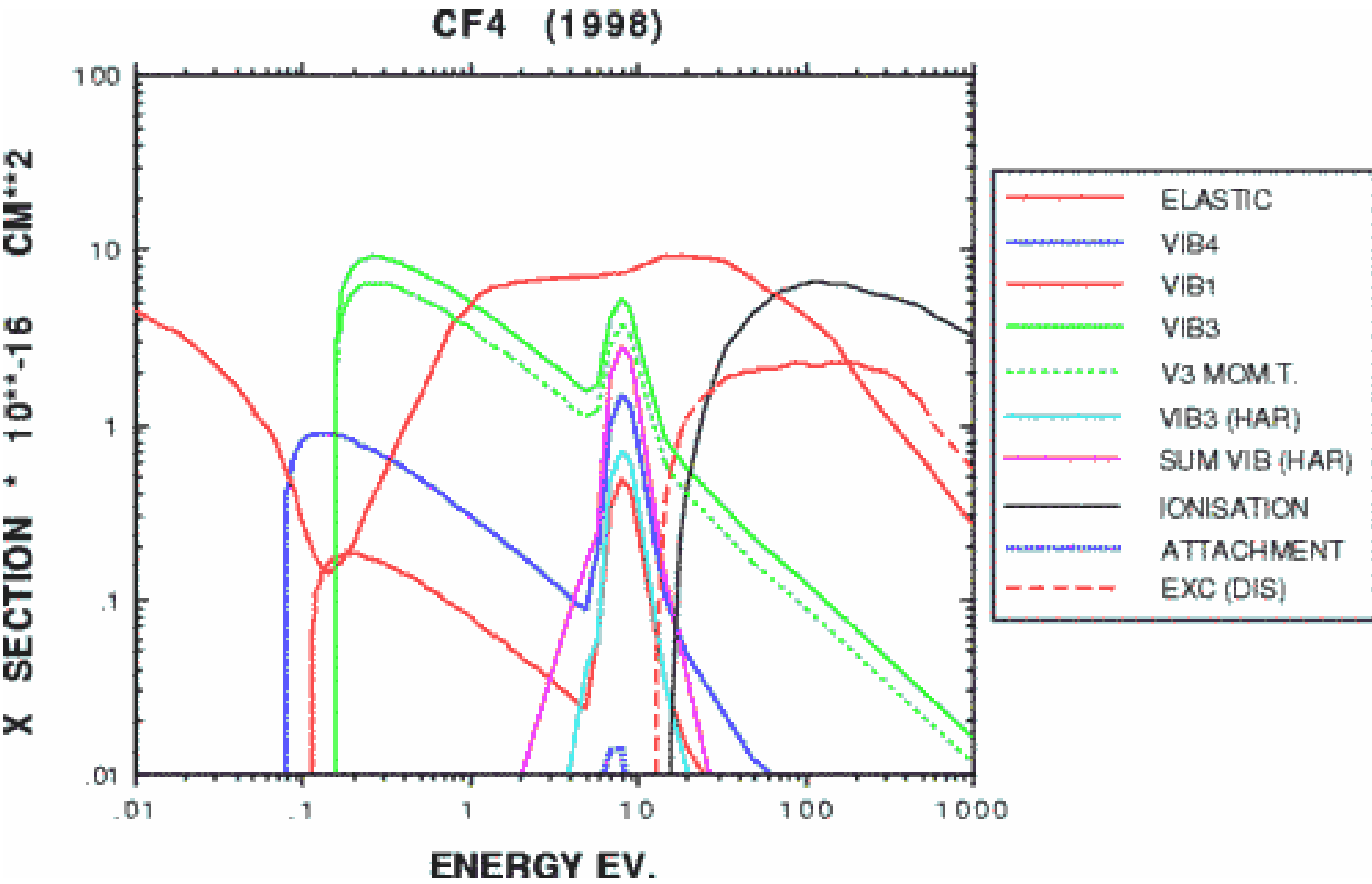


CO2 (2004)
T = 293 K
X SECTION * 10**-16 CM**2
ENERGY EV.
100
10
1
.1
.01
.01
.1
1
10
100
1000
ROT STATES
GLOBAL WARMING ?
V(010)
V(020)
V(100)
V(030+110)
V(001)
V(POLYAD3)
V(130+210)
V(POLYAD4)
V(POLYAD5)
V(POLYAD6)
V(POLYAD7)
V(POLYAD8)
V(POLYAD9)
V(SUM HIGH)
ELAST MT
ELAS VIB MT
EXC 7.9
EXC 8.9
EXC 10.5
EXC 12.2
EXC 13.2
EXC 15.0
IONS

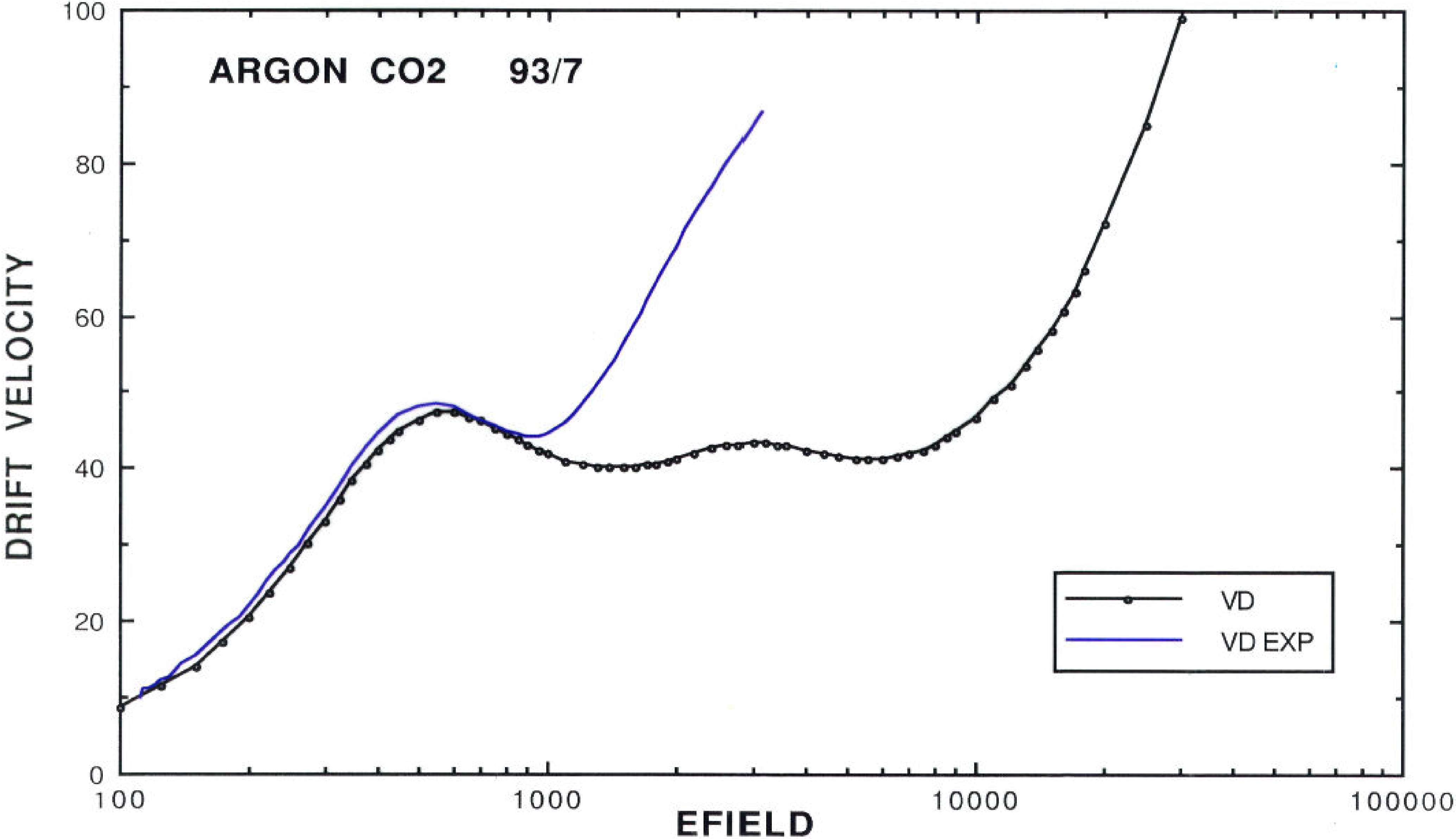

ARGON (2002)
X SECTION * 10**-16 CM**-2
100
10
1
.1
.01
.01
.1
1
10
100
1000
ENERGY EV.
ELAST. MT
ELAST. TOT
EXC S
EXC. P
EXC. D
IONS.
EXC. SUM

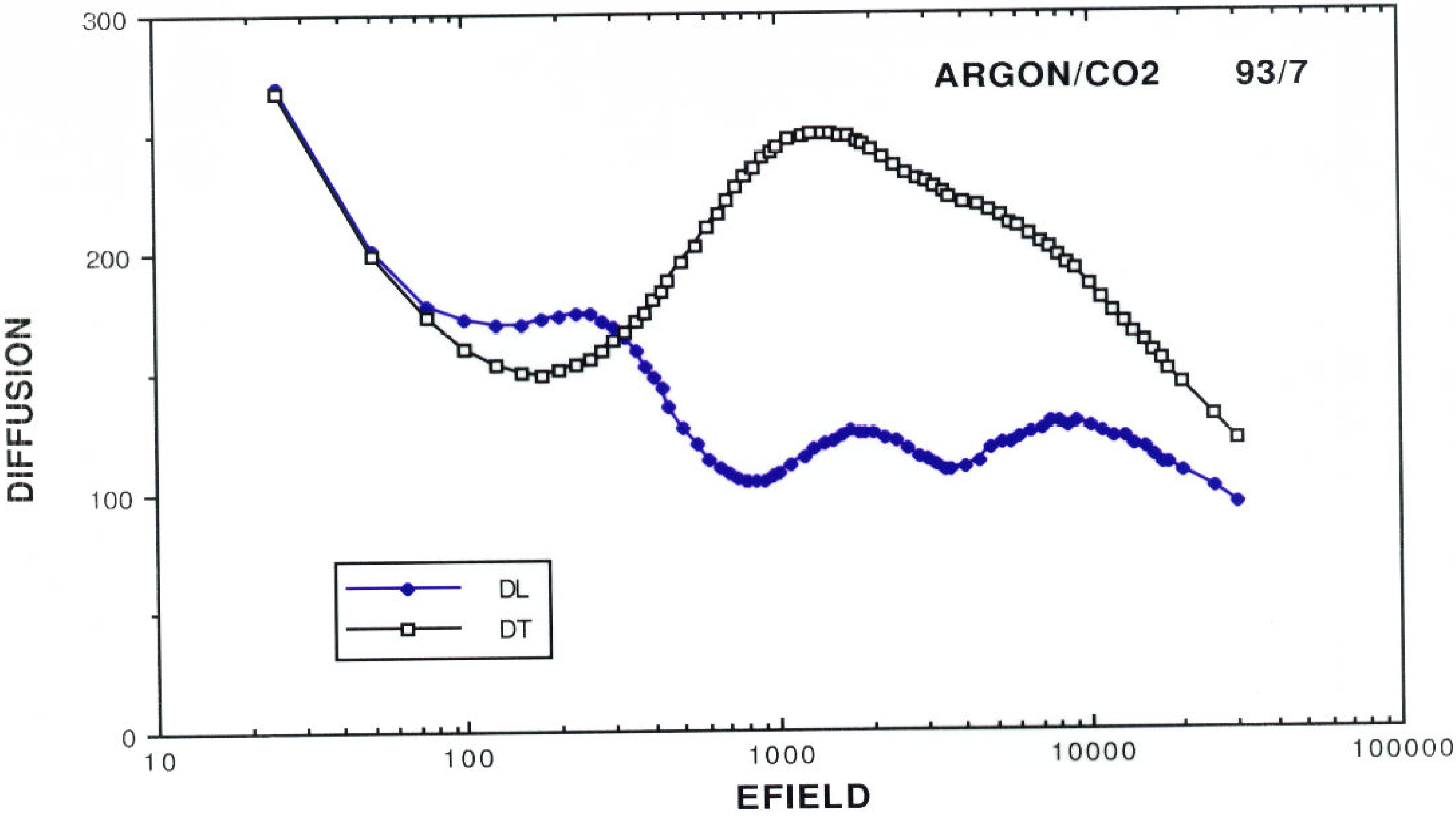


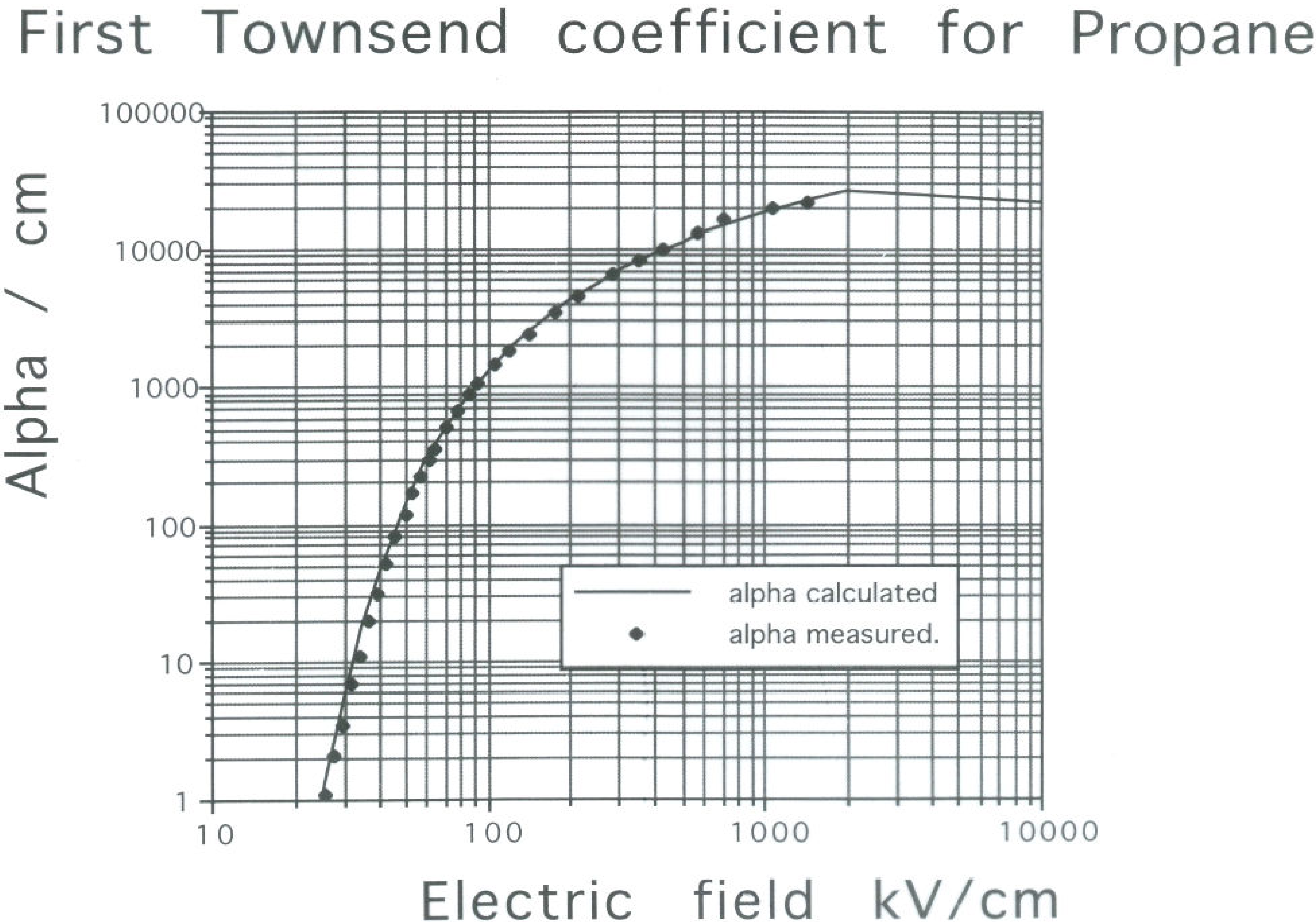
XENON (2002)
100
10
1
.1
.01
X SECTION * 10**-16 CM**2
.01
.1
1
10
100
1000
ENERGY EV.
ELAST. MT
EXC1
EXC2
EXC3
EXC4
ION
EXC SUM
ELAST. TOT

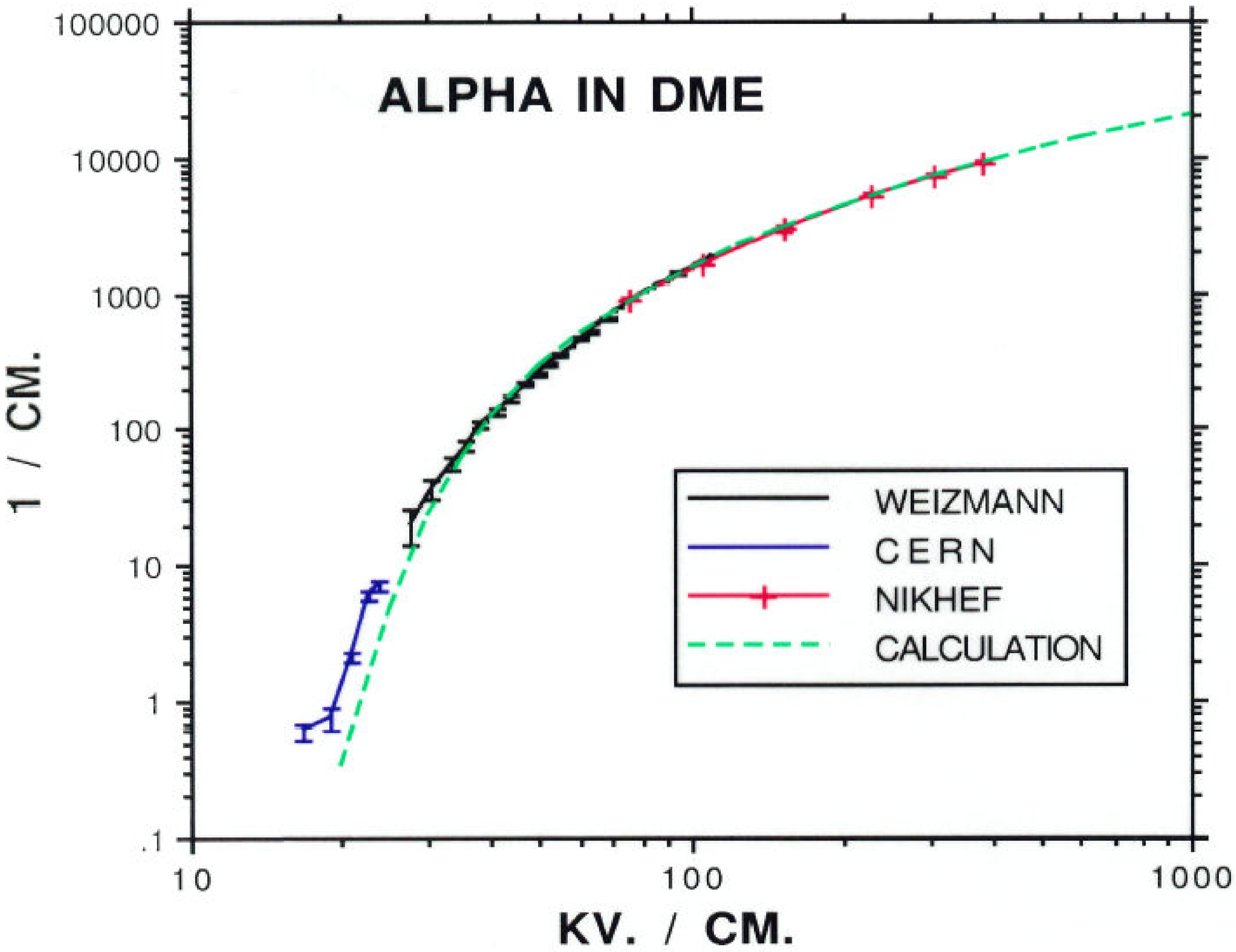


CF4 (1998)
X SECTION * 10**-16 CM**2
ENERGY EV.
100
10
1
.1
.01
.01
.1
1
10
100
1000
ELASTIC
VIB4
VIB1
VIB3
V3 MOM.T.
VIB3 (HAR)
SUM VIB (HAR)
IONISATION
ATTACHMENT
EXC (DIS)


ARGON CO2 93/7
DRIFT VELOCITY
EFIELD
0
20
40
60
80
100
100
1000
10000
100000
VD
VD EXP


ARGON/CO2 93/7
DIFFUSION
EFIELD
DL
DT
300
200
100
0
10
100
1000
10000
100000


First Townsend coefficient for Propane
Alpha / cm
100000
10000
1000
100
10
1
10
100
1000
10000
Electric field kV/cm
alpha calculated
alpha measured.



ALPHA IN DME
100000
10000
1000
100
10
1
.1
1 / CM.
10
100
1000
KV. / CM.
WEIZMANN
C E R N
NIKHEF
CALCULATION

TABLE OF EXPERIMENTAL AND CALCULATED TRANSPORT COEFICIENTS IN H2O

BRACKETS GIVE EXPERIMENTAL AND CALCULATION ERRORS ON THE LAST DIGITS.
CALCULATION ERRORS ARE STATISTICAL ERRORS FROM MONTE CARLO.

ELECTRIC FIELD IN TOWNSEND T=293 KELVIN

EFLD	VEXP	VCALC	DTEXP	DTCALC	DLEXP	DLCALC
2	0.452(4)	0.451(5)	0.0254	0.0254(2)	0.0254(25)	0.0250(20)
4	0.905(9)	0.914(7)	0.0254	0.0252(2)	0.0254(25)	0.0252(10)
8	1.82(1)	1.829(8)	0.0261	0.0257(2)	0.0264(25)	0.0260(15)
10	2.28(2)	2.293(8)	0.0262	0.0261(2)		0.0274(15)
16	3.69(3)	3.720(9)	0.0272	0.0276(2)	0.0285(28)	0.0292(15)
20	4.67(3)	4.71(1)	0.0280	0.0290(2)	0.0300(30)	0.0315(15)
24	5.72(4)	5.75(1)	0.0295	0.0310(2)	0.0340(34)	0.0360(20)
28	6.82(6)	6.86(1)	0.0325	0.0339(4)	0.0410(41)	0.0430(30)
32	8.10(7)	8.08(1)		0.0400(8)	0.0600(60)	0.0625(50)
40	11.35(9)	11.10(1)		0.105(2)	0.400(40)	0.310(20)
48	17.5(7)	16.9(1)		0.41(2)	2.0(2)	1.55(15)
56	29.0(9)	28.6(2)		0.95(2)	4.0(4)	3.5(2)
64	49.4(15)	48.5(4)	1.8	1.7(1)	4.6(5)	4.8(3)
72	74.0(20)	74.0(6)	2.3	2.1(1)	4.0(4)	4.8(3)
80	98.0(30)	99.0(8)	2.6	2.5(1)		4.3(2)
100	144(5)	146(2)	3.0	3.3(1)		3.3(1)
120	173(6)	176(2)	3.3	3.8(1)		3.1(1)
200	257(8)	255(2)	3.7	5.2(1)		4.0(1)
400		414(4)		7.1(2)		6.6(2)
1000		780(8)		13.4(3)		14.0(5)

ADDITIONAL TRANSPORT DATA: ALPHA AND ATT IN CM**-1 AT 760 TORR AND 293K
WR IS TOF DRIFT VELOCITY.

EFLD	ALPHA(EXP)	ALPHA(CALC)	ATT(EXP)	ATT(CALC)	WR
40			2(1)	3(2)	
48		0.2(1)	14(3)	19(1)	
56	4(2)	1.5(1)	56(10)	52(1)	
64	7(2)	5.4(1)	95(20)	87(2)	
72	12(2)	13(1)	110(10)	109(1)	
80	20(4)	23(1)	125(10)	122(1)	
100	55(4)	65(1)	130(10)	129(1)	
120	110(10)	125(5)	130(10)	126(5)	
200	485(20)	488(2)	100(10)	92(2)	285(8)
400	1625(50)	1648(2)		50(2)	517(8)
1000	4900(100)	4650(50)		20(2)	1100(8)