Improvements to magboltz and degrad data bases

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and

R51 CERN

Outline:

Need to improve data base for more accuracy:

1) Light emission
2) fano factors W and F
3) DE/DX and range
4) Cluster size and spacing for charged tracks
5) Better description of quenching

New Inputs:

1) Introduce all possible dissociative ionisation channels and ion charge states
2) Calculate neutral dissociation from oscillator strength data corrected for ionisation efficiency.

SUMMARY OF RECENT DATA BASE UPDATES:

Noble gases:

Helium: Ionisation :

He+ and He++ now have consistency between calculations and experimental measurements. Previously 10% difference ..

Ionisation energy =24.58739 ev

49 levels used in data base all have consistency between experiment and theory at the 1% level.

levels are between 19.81961 and 24.49308 ev

The remaining levels between 24.49308 and the ionisation energy are approximated by a level at 24.50708 ev with the remaining oscillator strength from the sum rule of F=0.00440 which is 1.5% of the total oscillator strength

Neon: Ionisation: Ne + ionisation energy =21.56454 ev

Ne 2+

Ne 3+

Ne Kshell

45 excitation levels used from 16.61907 to 21.11401 ev

The remaining oscillator strength between 21.11401 and the ionisation energy is approximated by two levels at : 21.14638 ev s-state

21.18286 ev d-state

these contain 9% of the remaining oscillator strength from the TRK sum rule

Argon : ionisation: ionisation energy = 15.75961 ev

Ar +

Ar 2+

Ar 3+

Ar K shell

Ar L1 shell

Ar L2 shell

Ar L3 shell

44 excitation levels between 11.548 and 15.374 ev

The remaining oscillator strength between 15.374 and the ionisation energy is approximated by a level at 15.66 ev with 14% of the total oscillator strength from the TRK sum rule.

Krypton : ionisation: Ionisation energy 13.9996 ev

Kr +

Kr 2+

Kr 3+

Kr 4+

Kr K shell

Kr L1 shell

Kr L2 shell

Kr L3 shell

Kr M1 shell

Kr M2 shell

Kr M3 shell

Kr M4 shell

Kr M5 shell

51 excitation levels between 9.9152 and 13.4365 ev

The remaining oscillator strength beteween 13.4365 and the ionisation energy is approximated by a level at 13.6 ev with 11% of the total oscillator strength from the TRK sum rule.

Xenon : Ionisation : ionisation energy 12.129843 ev

Xe +
Xe 2+
Xe 3+ Xe 4+ Xe 5+ Xe 6+
Xe K shell
Xe L1 shell
Xe L2 shell
Xe L3 shell
Xe M1 shell
Xe M2 shell
Xe M3 shell
Xe M4 shell
Xe M5 shell

50 levels between 8.3153155 and 11.993947 ev

The remaining oscillator strength between 11.993947 and the ionisation energy is approximated by a level at 12.0ev with 5% of the oscillator strength from the TRK sum rule..

Methane : Ionisation : ionisation energy 12.65 ev

CH_4 +

CH_3 +

CH_2 +

H +

CH +

CH +* < PRODUCED MAINLY IN EXCITED STATE

C +

CH_n ++

H_2 +

C K shell

Dissociation: LIGHT EMISSION:

CH(A2delta > GS)

CH(B2sigma > GS)

H(Alpha > GS)

H(Beta > GS)

8 VIBRATIONAL LEVELS AND 26 EXCITATION(DISSOCIATIVE) LEVELS

FROM OSCILLATOR STRENGTH USE LEVELS BETWEEN 7.50 AND 15.75 EV

UNACCOUNTED ENERGY LOSSES TO EXCITED IONS (NOT IN GS)

GIVEN BY EFFECTIVE LEVEL AT 16 EV

SUPEREXCITED STATES AT 20.5 AND 22 EV ALSO INCLUDED.

ISOBUTANE: IONISATION IONISATION ENERGY 10.67 ev

NO EXPERIMENTALLY MEASURED DISSOCIATIVE IONISATION
USE ONLY C4H10 + IONISATION
AND ASSUME ANOTHER BREAKUP CHANNEL AT 17 ev

24 LEVELS: 9 VIBRATIONS AND 15 EXCITATIONS.
USED SOME MEASURED OSCILLATOR STRENGTHS BETWEEN
7.2 AND 13.5 EV TO GIVE DISSOCIATIVE CHANNELS

NEED MORE EXPERIMENTAL DATA FROM ELECTRON SCATTERING
IN ORDER TO IMPROVE THE ISOBUTANE SIMULATION……

CF4 : IONISATION : IONISATION ENERGY

CF_3^+

CF_2^+

CF_3^{++}

C^+

F^+

CF_2^{++}

(C^+ , F^+)

(CF^+ , F^+)

(CF_2^+ , F^+)

(CF_3^+ , F^+)

C K shell

F K shell

Dissociative Attachment and 46 Inelastic levels:

10 Vibrations and 36 neutral dissociations

Light emission in argon mix from $CF_3^* > CF_3$ + photon

Dissociation from oscillator strength between 11.5 and 20 ev

Non dipole dissociation in 3 levels and adjusted to fit Townsend gain

CO_2 : ionisation : **ionisation energy : 13.776ev**

- CO_2 + (GS)
- CO_2 +(A2Pi)
- CO_2 +(B2Sigma)
- O +
- CO +
- C +
- CO_2 ++
- C ++
- O ++
- C K shell
- O K shell

76 ROTATIONAL LEVELS 19 VIBRATIONAL LEVELS

125 EXCITATION LEVELS

LEVELS ABOVE 13.776 ALL DISSOCIATIVE

CROSS-SECTIONS FROM OSCILLATOR STRENGTHS FOR DIPOLE LEVELS

HYDROGEN : IONISATION : IONISATION ENERGY 15.418 EV

H_2 +

H +

107 LEVELS : 8 ROTATIONS 4 VIBRATIONS

95 EXCITATION AND DISSOCIATIONS

OSCILLATOR STRENGTHS KNOWN FOR MANY INDIVIDUAL LEVELS

MANY LIGHT EMITTING LEVELS :

LYMAN AND WERNER BAND EXCITATIONS CALCULATED FOR EACH VIBRATIONAL STATE WITHIN BAND.

NITROGEN: IONISATIONS : IONISATION ENERGY 15.581 EV

N2 + (GS)
N2 + (V>0)
N2 + (A2Pi V=O)
N2 + (A2Pi V=1)
N2 + (A2Pi V>1)
N2 + (B2sigma)
N2 + (C2sigma)
N +
(N + , N *)
N + *
N ++
(N + , N +)
N K shell

127 EXCITATION LEVELS : 76 ROTATIONAL LEVELS 16 VIBRATIONAL LEVELS

35 LEVELS WHICH HAVE ONLY SMALL DISSOCIATIVE FRACTIONS BELOW IONISATION THRESHOLD.
POOR QUENCHER GAS (LOTS OF LIGHT EMISSION AND LOW DISSOCIATION)

OXYGEN : IONISATION : **IONISATION ENERGY 12.071 ev**

O_2 + (GS)
O_2 + (A Pi)
O_2 + (B4sigma)
O +
(O + , O +)
O ++
(O ++ , O +)
O K shell

3 BODY ATTACHMENT
2 BODY DISSOCIATIVE ATTACHMENT

148 LEVELS : 48 ROTATIONAL LEVELS
23 VIBRATIONAL LEVELS
77 EXCITATION LEVELS MAINLY DISSOCIATIVE
OSCILLATOR STRENGTH FROM EXPERIMENT USED FOR DISSOCIATIVE X-SECTIONS

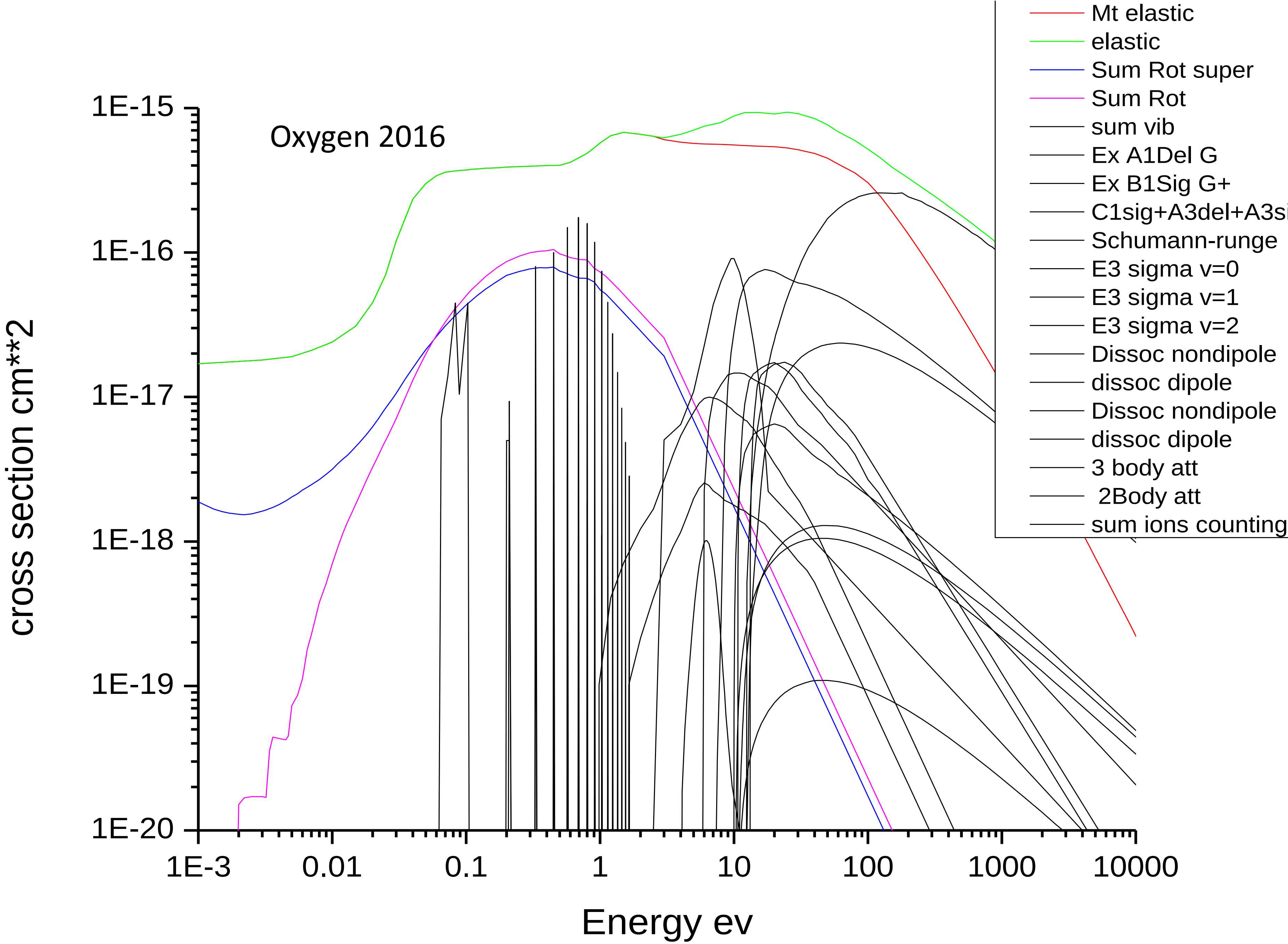
NB (DISSOCIATION ENERGY IN OXYGEN IS ONLY 5 EV)

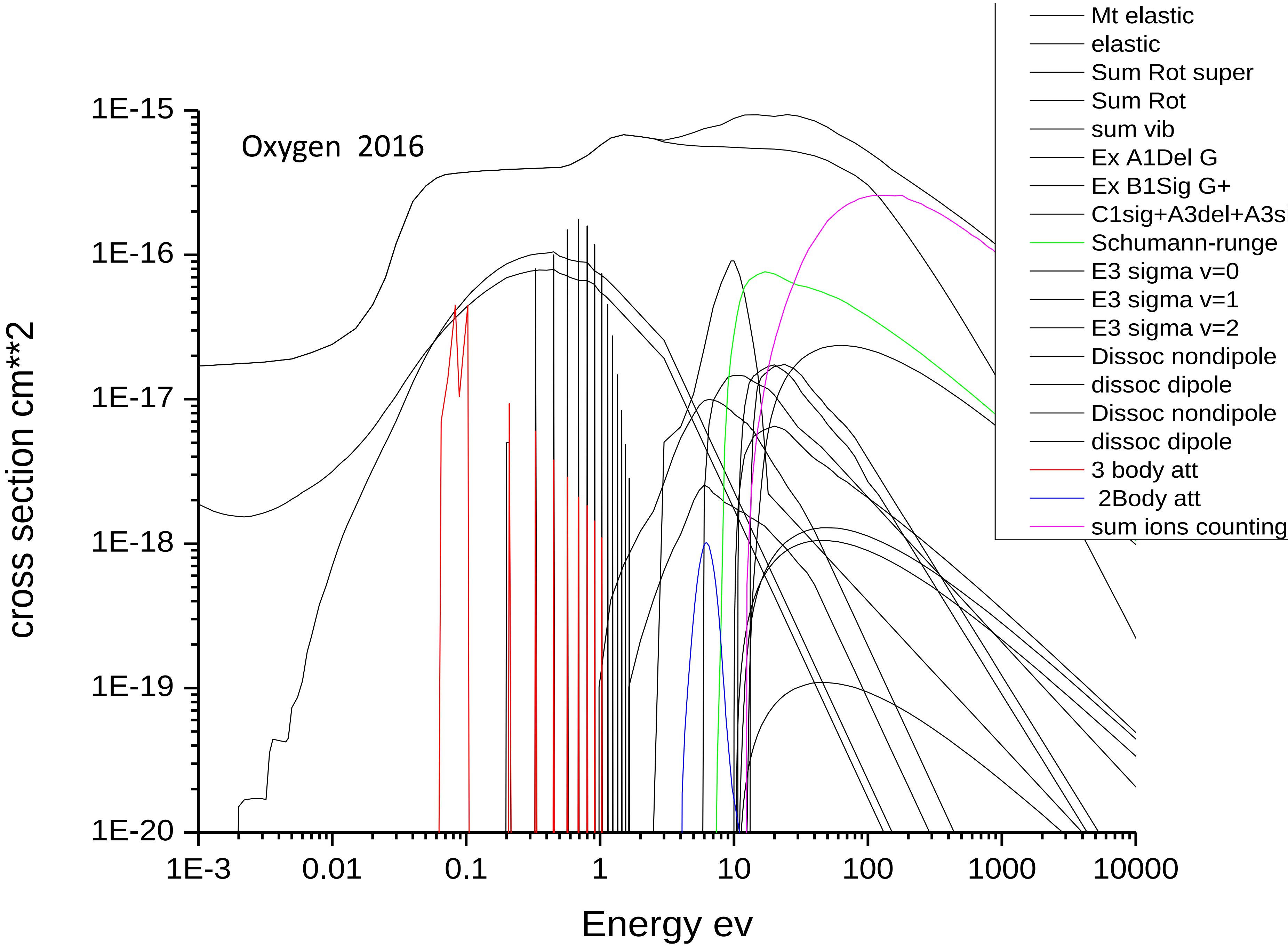
Most recent update was oxygen :

Old data base contained incorrect rotational x-sections which made the 3 –body attachment inaccurate.

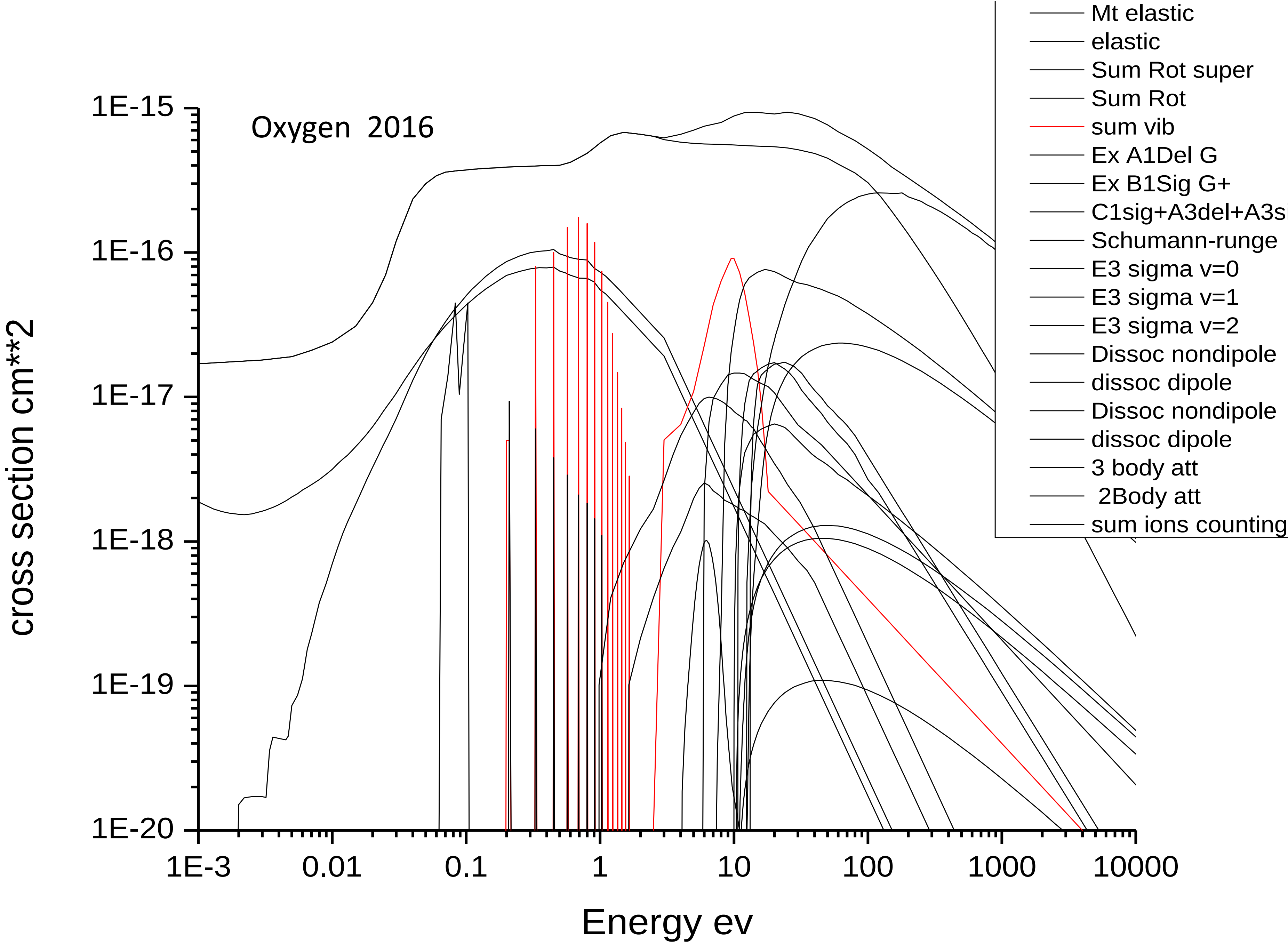
The new data base now also has the correct temperature dependence of the 3-body attachment

The oxygen subroutine now contains a scaling factor that is clearly indicated in the code which can be changed from 1.0 to any value to allow the rate to be adjusted for any gas mixture. The program then needs recompiling…

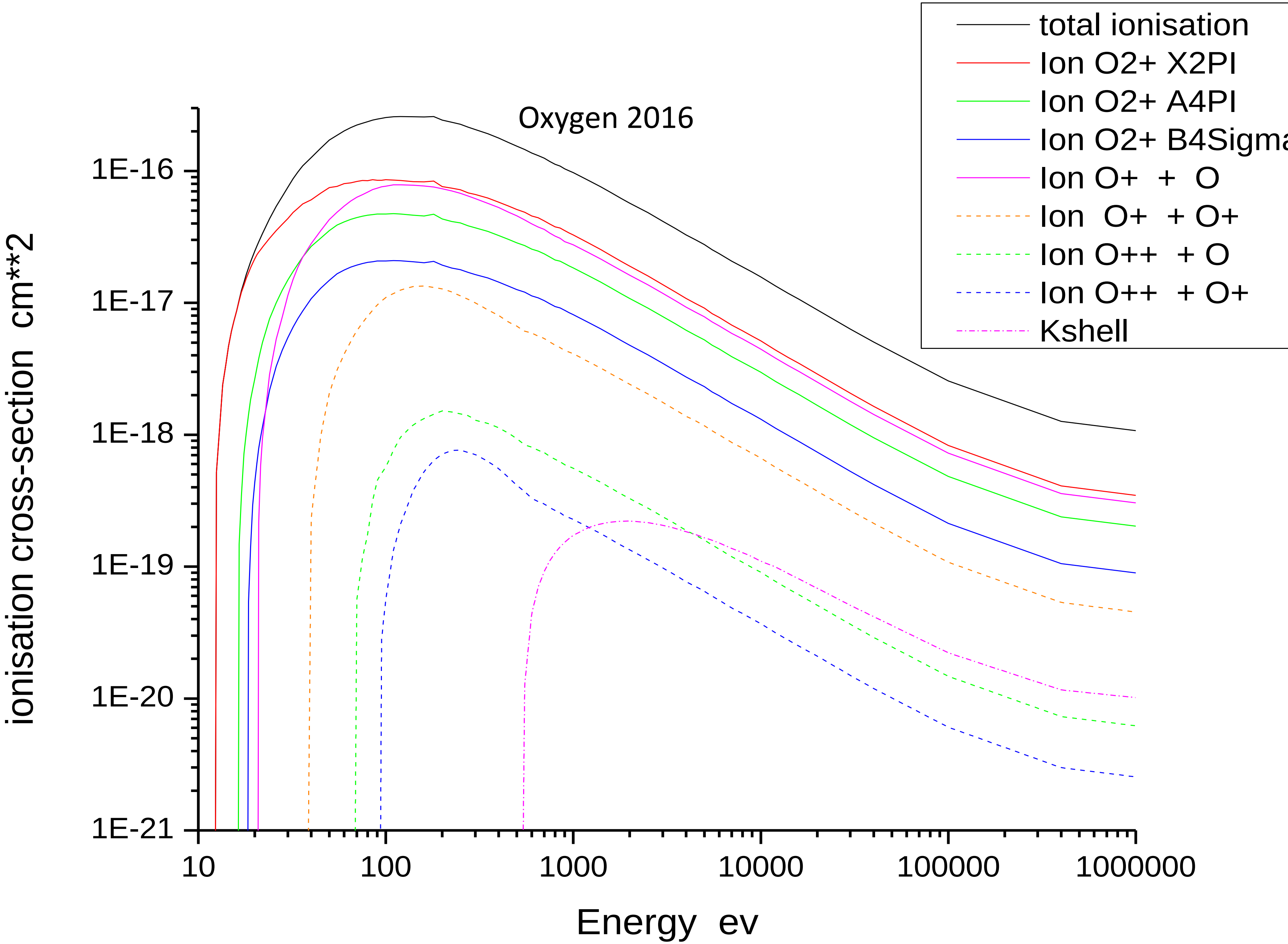

Oxygen 2016
Mt elastic
elastic
Sum Rot super
Sum Rot
sum vib
Ex A1Del G
Ex B1Sig G+
C1sig+A3del+A3si
Schumann-runge
E3 sigma v=0
E3 sigma v=1
E3 sigma v=2
Dissoc nondipole
dissoc dipole
Dissoc nondipole
dissoc dipole
3 body att
2Body att
sum ions counting
1E-15
1E-16
1E-17
1E-18
1E-19
1E-20
cross section cm**2
1E-3
0.01
0.1
1
10
100
1000
10000
Energy ev



Oxygen 2016
cross section cm**2
Energy ev
1E-15
1E-16
1E-17
1E-18
1E-19
1E-20
1E-3
0.01
0.1
1
10
100
1000
10000
Mt elastic
elastic
Sum Rot super
Sum Rot
sum vib
Ex A1Del G
Ex B1Sig G+
C1sig+A3del+A3si
Schumann-runge
E3 sigma v=0
E3 sigma v=1
E3 sigma v=2
Dissoc nondipole
dissoc dipole
Dissoc nondipole
dissoc dipole
3 body att
2Body att
sum ions counting



Oxygen 2016
cross section cm**2
Energy ev
1E-15
1E-16
1E-17
1E-18
1E-19
1E-20
1E-3
0.01
0.1
1
10
100
1000
10000
Mt elastic
elastic
Sum Rot super
Sum Rot
sum vib
Ex A1Del G
Ex B1Sig G+
C1sig+A3del+A3si
Schumann-runge
E3 sigma v=0
E3 sigma v=1
E3 sigma v=2
Dissoc nondipole
dissoc dipole
Dissoc nondipole
dissoc dipole
3 body att
2Body att
sum ions counting



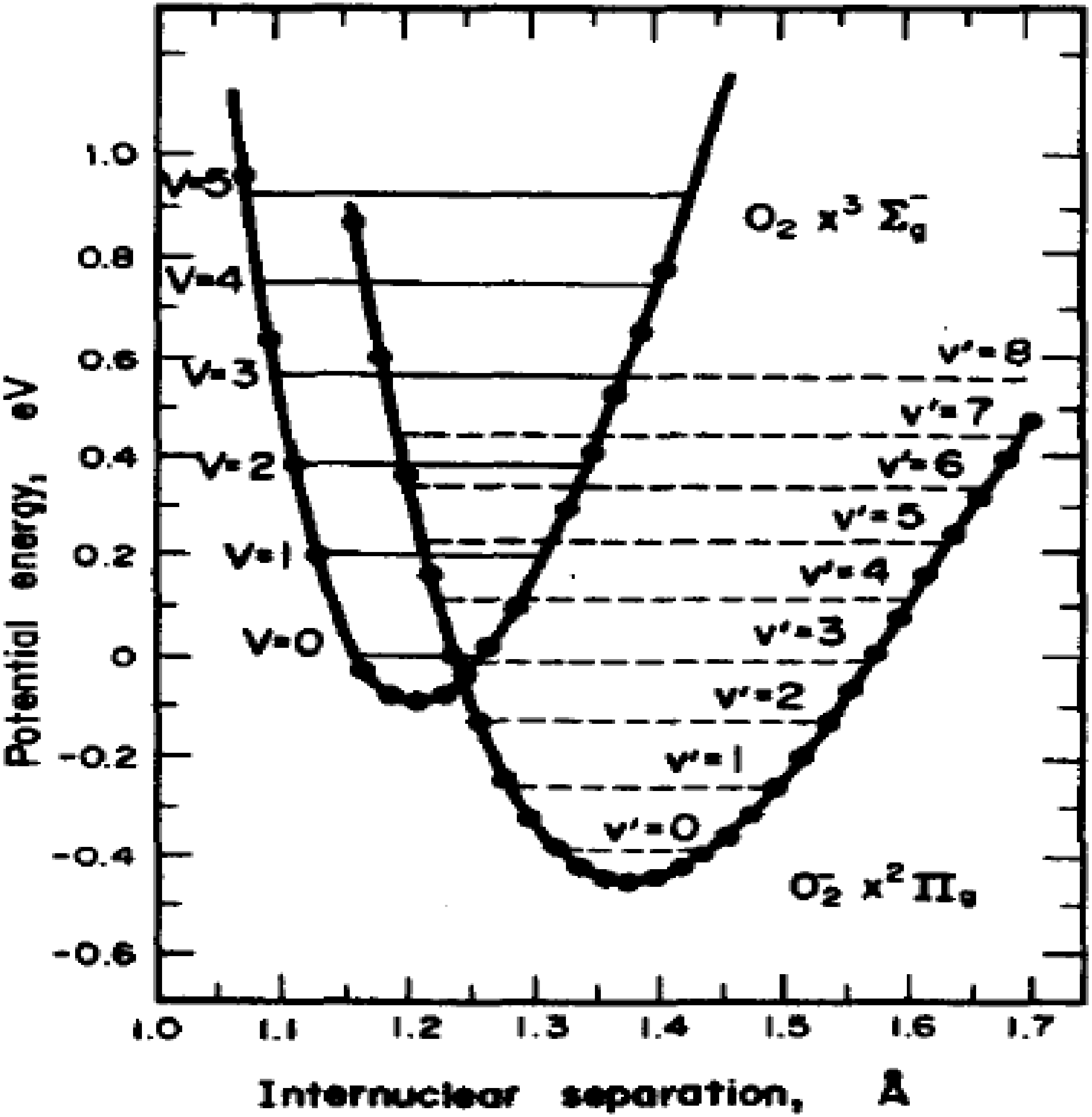
Oxygen 2016
total ionisation
Ion O2+ X2PI
Ion O2+ A4PI
Ion O2+ B4Sigma
Ion O+ + O
Ion O+ + O+
Ion O++ + O
Ion O++ + O+
Kshell
ionisation cross-section cm**2
1E-16
1E-17
1E-18
1E-19
1E-20
1E-21
10
100
1000
10000
100000
1000000
Energy ev

Table 1
Three-body rate constants at about 300 K ($\times 10^{-30}$ cm^6/s)

M	This work	Other works	
O_2	2.3 ± 0.2 a)	1.7	[4]
		1.9	e)
		2.0	[5]
		2.1	[9,11]
		2.2	[10]
		2.3	f)
		2.8	[3]
		3	g)
H_2	0.48 ± 0.03 b)		
D_2	0.140 ± 0.005 b)		
He	0.033 ± 0.003	0.03	[3]
		0.07	[2]
Ne	0.023 ± 0.003		
Ar	0.05 ± 0.01		
Kr	0.05 ± 0.01		
Xe	0.085 ± 0.005		
N_2	0.085 ± 0.003 c)	0.11	[2]
		0.06	[3]
		0.26	[4]
		0.15	f)
		0.078	[15]
CH_4	0.34 ± 0.01 d)	0.2	[32]
C_2H_4	~3	2.3	[1]
		3.1, 3.4	[6]
		1.7	[7]
		2.5	h)
		1.5	[15]
C_2H_6	1.7 ± 0.1	1.5	[15]
C_3H_8	3.3 ± 0.2		
n-C_4H_{10}	~5		
n-C_5H_{12}	7.9 ± 0.4		
neo-C_5H_{12}	8.0 ± 0.7		
n-C_6H_{14}	8.1 ± 0.4		
C_6H_6		18	[7]
CH_3OH	11 ± 2	9~10	[7], h)
C_2H_5OH	18		
CO_2		~3	[5,10], f), h)
H_2O		14	[5,6], h)
H_2S		10	[7]
NH_3		7	[7], h)
CH_3COCH_3		>35	[7]
		27	h)

a) This is an average of the values obtained by the present authors previously (refs. [18,19]).
b) This is taken from ref. [19].
c) This is taken from ref. [18].
d) This is an effective value, see text.
e) M.N. Hirsh and P.N. Eisner, Bull. Am. Phys. Soc. 8 (1963) 58.
f) H. Hackam and J.J. Lennon, Proc. Phys. Soc. 86 (1965) 123.
g) V.B. Brodskii and S.E. Zagik, ZhTF 36 (1966) 672 [English Transl., Soviet Phys.-Tech. Phys. 11 (1966) 498].
h) L. Bouby, F. Fiquet-Fayard and Y. LeCoat, Int. J. Mass Spectrom. Ion Phys. 3 (1970) 439.
i) A. Zastawny, Acta Physica Polonica A46 (1974) 39.

H.Shimamori and Y.hatano Chem.Phys.21(1977)187



Levels above v'=4
In the oxygen
negative ion
vibrational
band
can be
collisionally
stabilised

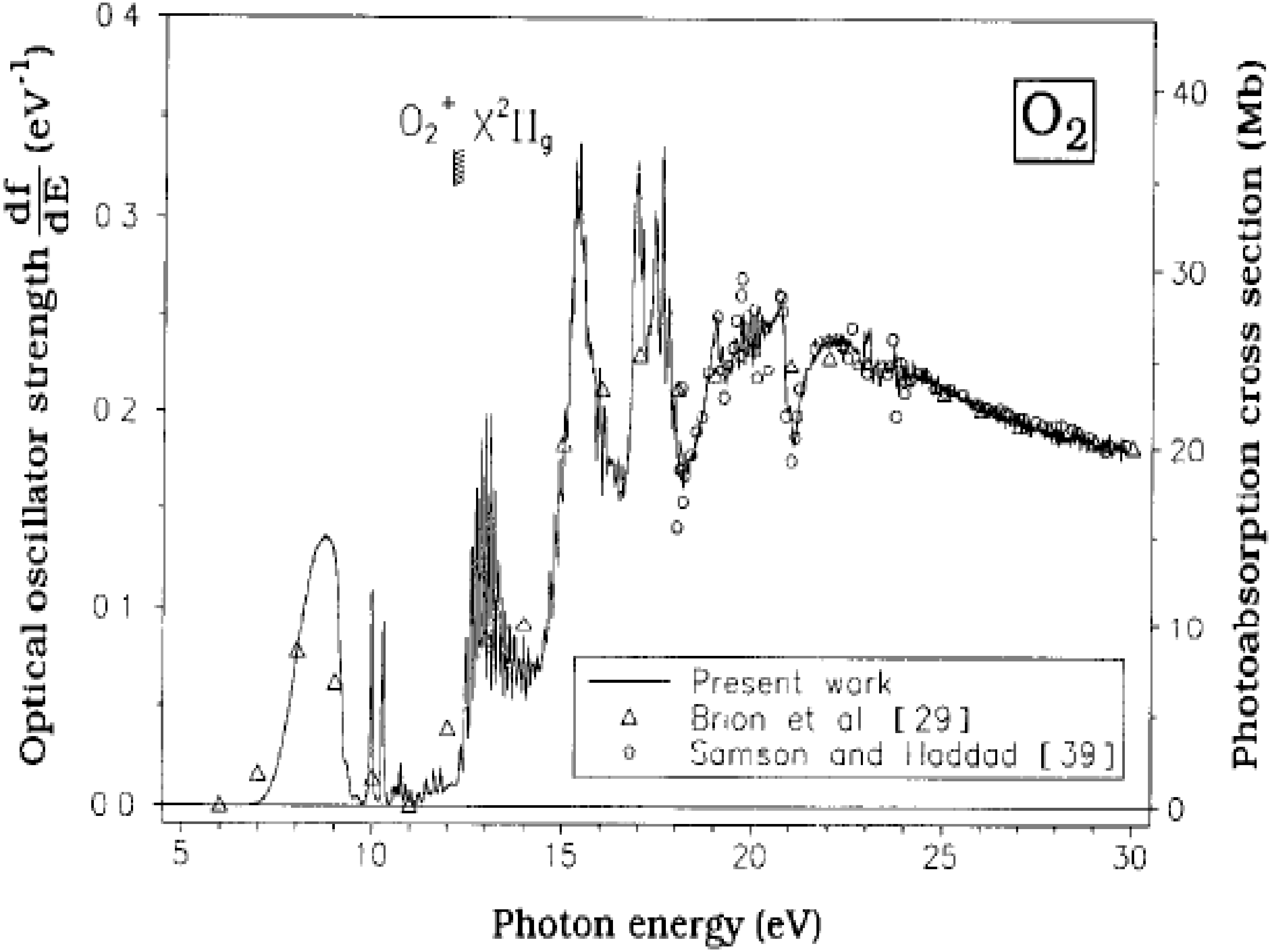


Fig. 1. Absolute oscillator strengths for the photoabsorption of molecular oxygen in the energy region 5–30 eV measured resolution dipole (e, e) spectrometer (fwhm = 0.048 eV).

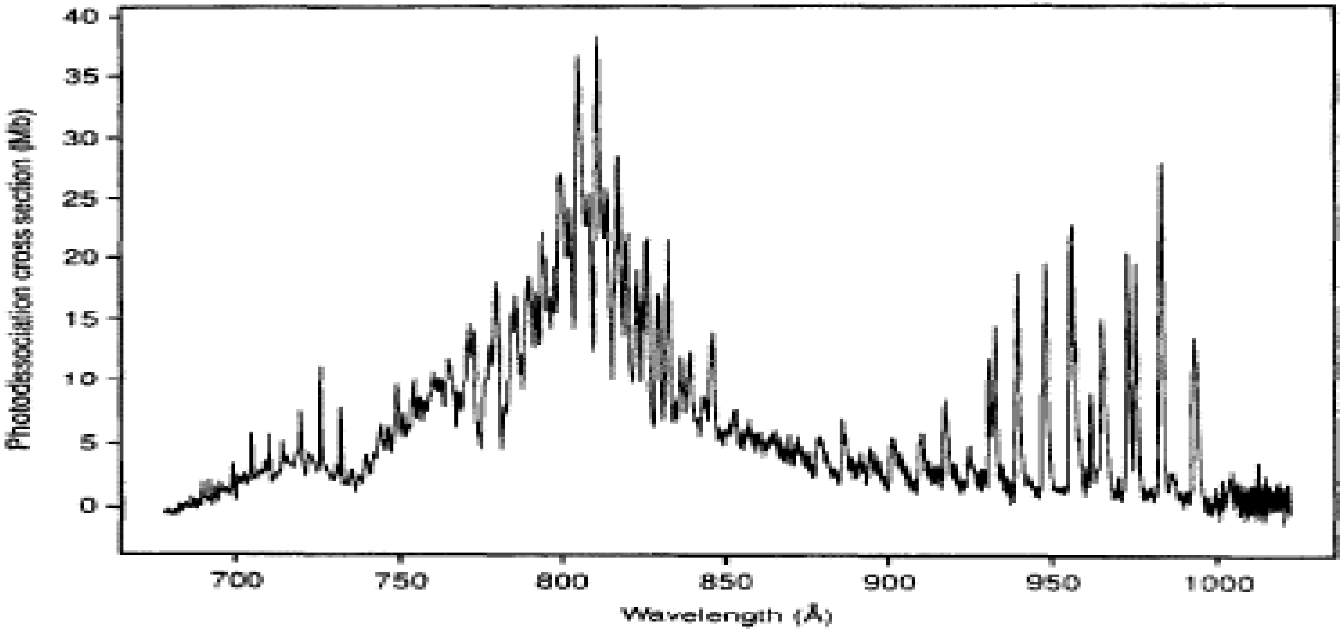


Fig. 8. The absolute photodissociation cross section of oxygen.

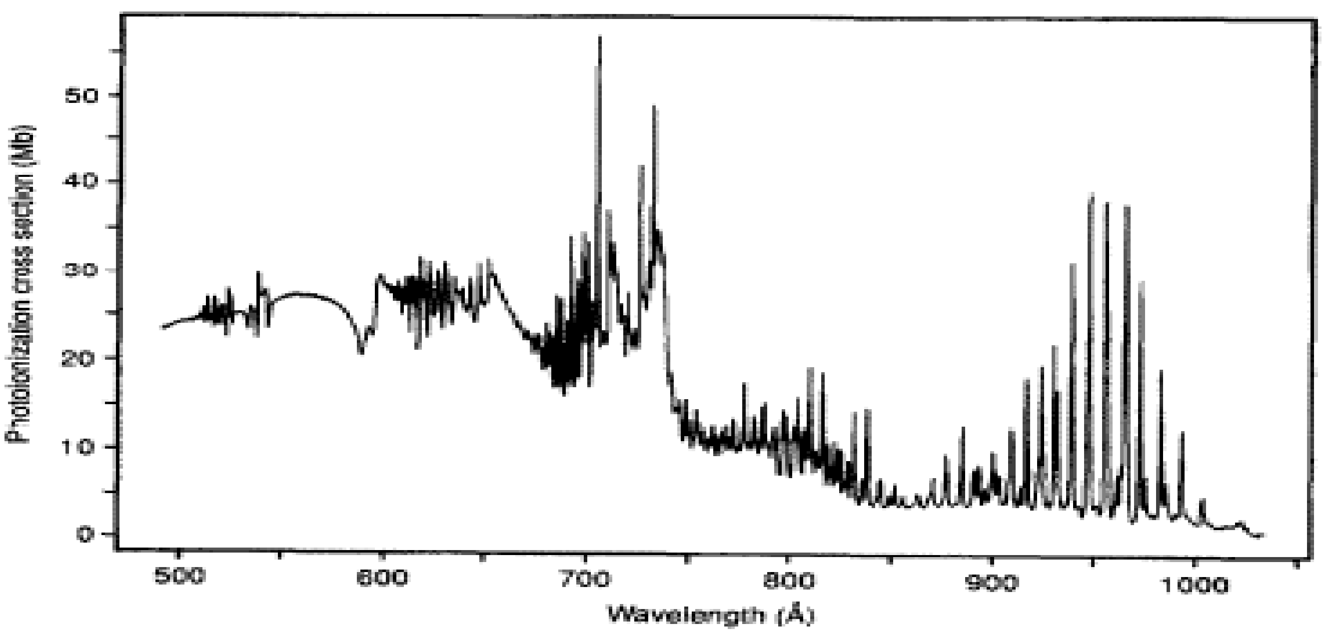
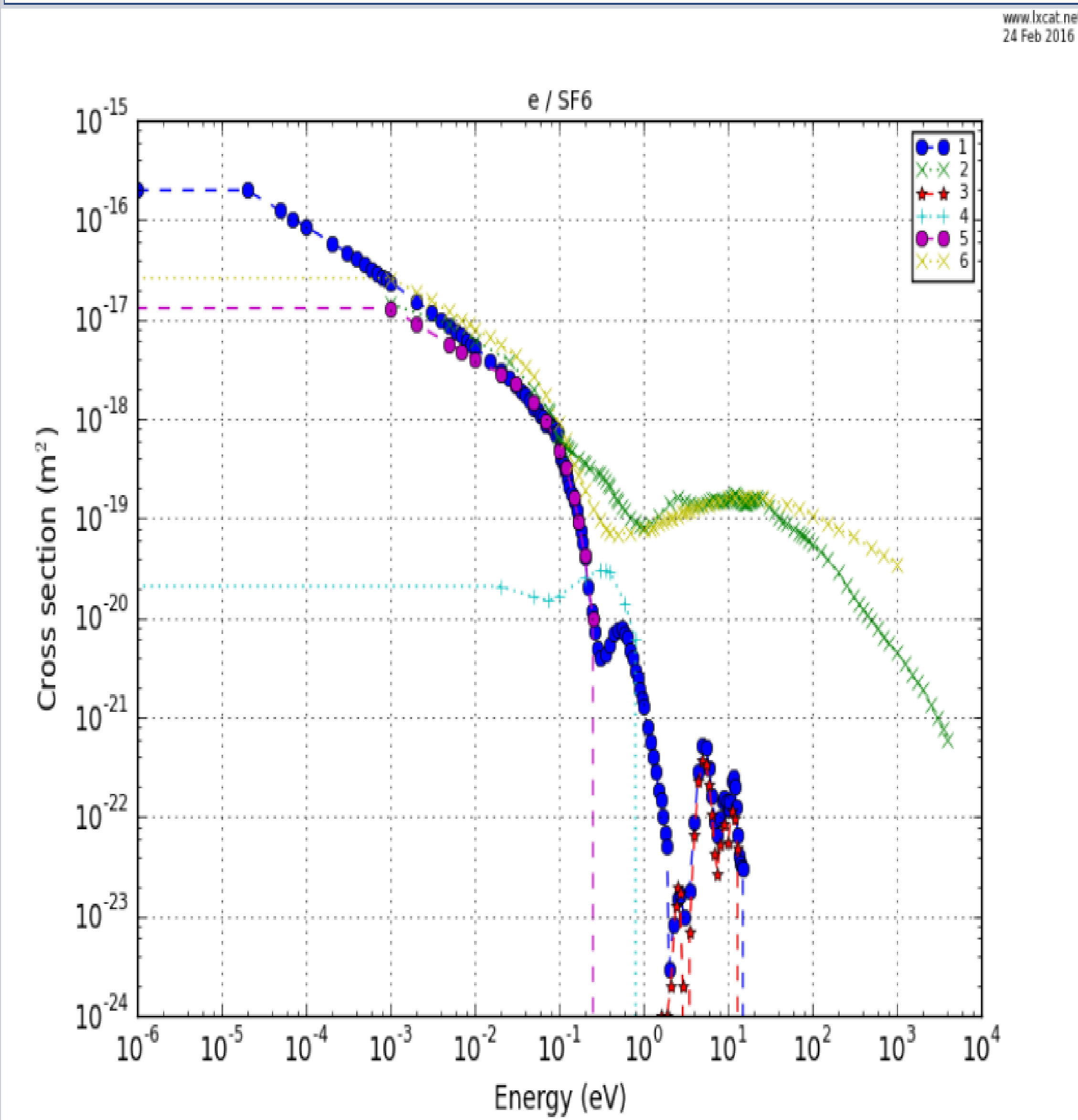


Fig. 9. The absolute photoionization cross section of oxygen.

LXCAT web site SF6 attachment

Cross section

GO BACK | KEEP WINDOW AND GO BACK | RESCALE IN NEW WINDOW | DOWNLOAD: TXT | PNG | XML | ZIP



Biagi-v8.3 (Compilation of electron cross sections used by S.F. Biagi)

Data Group [Mbltz version 10.6]

e / SF6

1. Attachment E + SF6 → sum of attachment processes (E = 0 eV, complete set) | Updated: 24 February 2016 13:22.

2. Elastic E + SF6 → E + SF6 (m/M = 0.0000037, complete set) | elastic momentum transfer. Updated: 23 February 2016 18:00.

Phelps database

Data Group [SF6]

e / SF6

3. Attachment E + SF6 → SF4$^-$+F2 (E = 0 eV, complete set) | Attachment TO FORM F-, F2-, AND SF4-. CHANTRY 2/78. Updated: 29 March 2010.

4. Attachment E + SF6 → SF5$^-$+F (E = 0 eV, complete set) | Attachment TO FORM SF5- KLINE ET AL. Updated: 29 March 2010.

5. Attachment E + SF6 → SF6$^-$ (E = 0 eV, complete set) | Attachment TO FORM SF6- PHELPS 5/85. Updated: 13 March 2010.

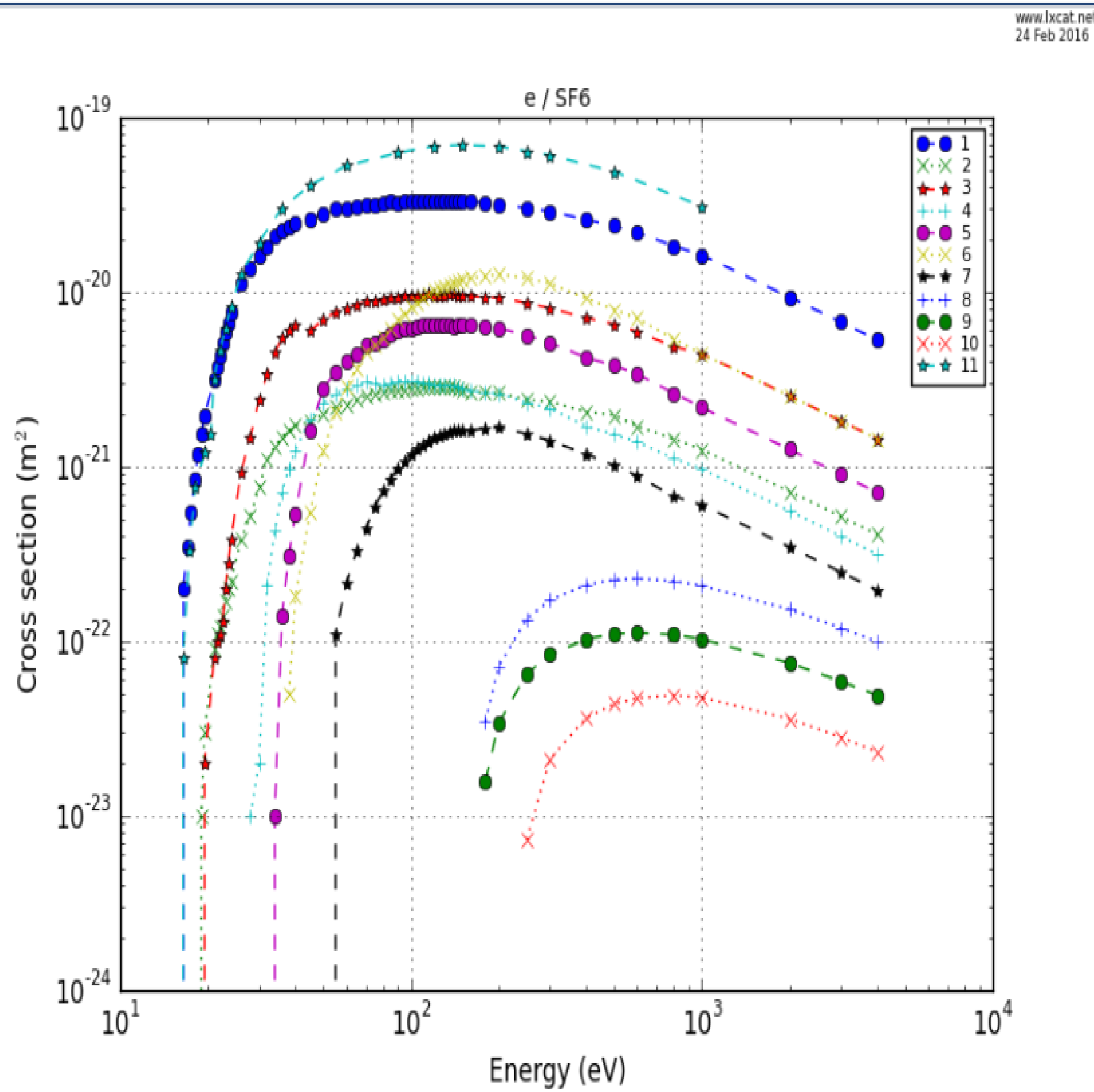
6. Effective E + SF6 → E + SF6 (m/M = 0.0000037, complete set) | Updated: 6 June 2011.

LXCAT web site

SF6 ionisation

Cross section

GO BACK | KEEP WINDOW AND GO BACK | RESCALE IN NEW WINDOW | DOWNLOAD: TXT | PNG | XML | ZIP



Biagi-v8.3 (Compilation of electron cross sections used by S.F. Biagi)

Data Group [Mbltz version 10.6]
e / SF6

1. Ionization E + SF6 → E + E + IONISATION SF5 + (E = 15.67 eV, complete set) | Updated: 23 February 2016 15:23.
2. Ionization E + SF6 → E + E + IONISATION SF4 + (E = 18.5 eV, complete set) | Updated: 23 February 2016 15:23.
3. Ionization E + SF6 → E + E + IONISATION SF3 + (E = 18.8 eV, complete set) | Updated: 23 February 2016 15:30.
4. Ionization E + SF6 → E + E + IONISATION SF2 + (E = 27 eV, complete set) | Updated: 23 February 2016 15:26.
5. Ionization E + SF6 → E + E + IONISATION SF + (E = 31 eV, complete set) | Updated: 23 February 2016 15:27.
6. Ionization E + SF6 → E + E + IONISATION SUM OF: S + AND F + (E = 37 eV, complete set) | Updated: 23 February 2016 15:27.
7. Ionization E + SF6 → E + E + IONISATION SUM OF (SF3 SF2 SF)2+ (E = 46.5 eV, complete set) | Updated: 23 February 2016 15:27.
8. Ionization E + SF6 → E + E + IONISATION SULFUR L3 SHELL (E = 164.16 eV, complete set) | Updated: 23 February 2016 15:28.
9. Ionization E + SF6 → E + E + IONISATION SULFUR L2 SHELL (E = 165.36 eV, complete set) | Updated: 23 February 2016 15:31.
10. Ionization E + SF6 → E + E + IONISATION SULFUR L1 SHELL (E = 230.9 eV, complete set) | Updated: 24 February 2016 13:28.

Phelps database

Data Group [SF6]
e / SF6

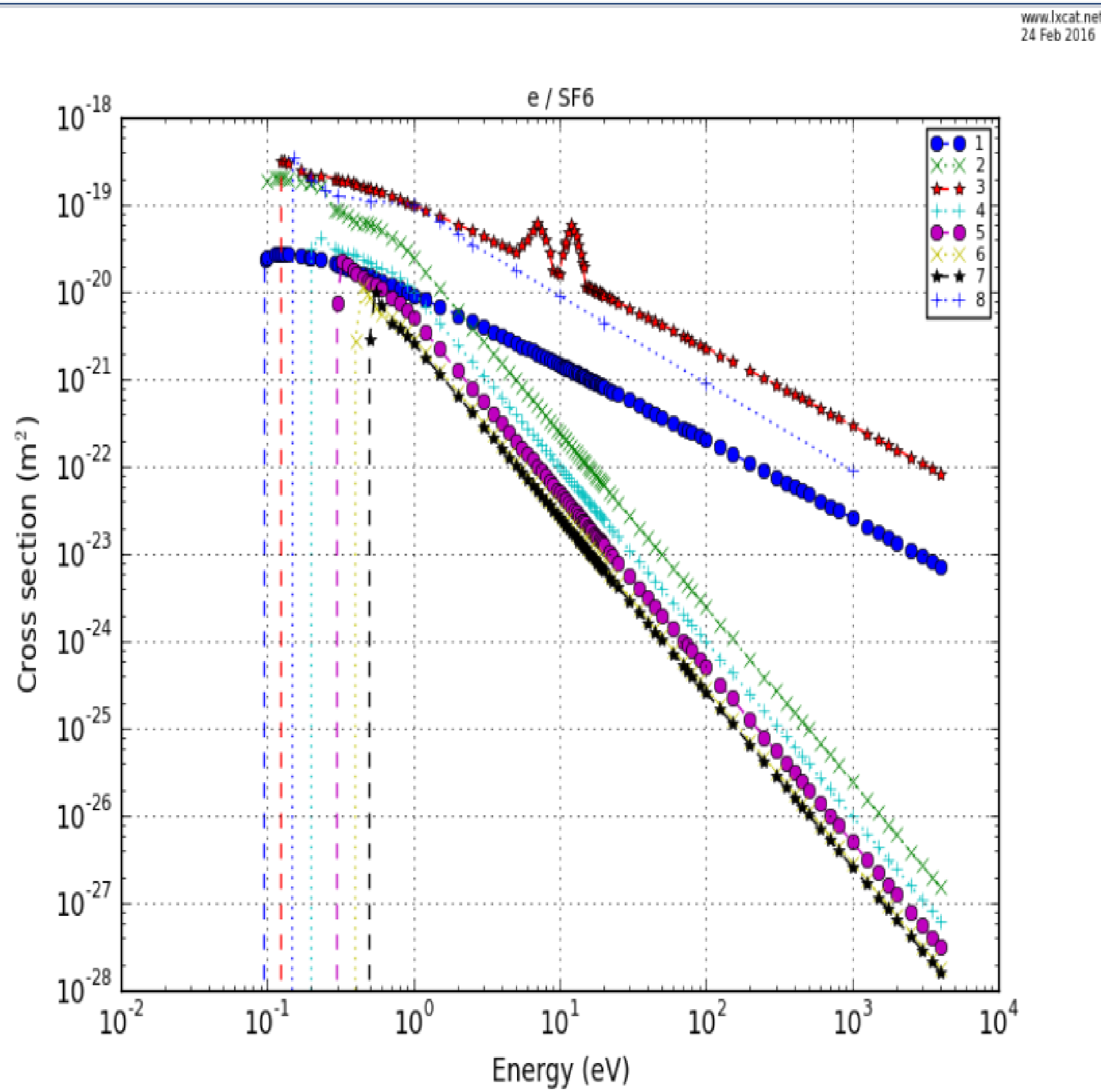
11. Ionization E + SF6 → E + E + $SF6^{+}$ (E = 15.7 eV, complete set) | Total ionization, CHANTRY

LXCAT web site

SF6 vibrations

Cross section

GO BACK | KEEP WINDOW AND GO BACK | RESCALE IN NEW WINDOW | DOWNLOAD: TXT | PNG | XML | ZIP



Biagi-v8.3 (Compilation of electron cross sections used by S.F. Biagi)

Data Group [Mbltz version 10.6]
e / SF6

1. Excitation E + SF6 → E + SF6(v4) (E = 0.076253 eV, complete set) | anisotropic. Updated: 23 February 2016 18:01.
2. Excitation E + SF6 → E + SF6(V1) (E = 0.096032 eV, complete set) | Updated: 23 February 2016 18:02.
3. Excitation E + SF6 → E + SF6(v3) (E = 0.11754 eV, complete set) | anisotropic. Updated: 23 February 2016.
4. Excitation E + SF6 → E + SF6(2v1) (E = 0.192064 eV, complete set) | Updated: 23 February 2016.
5. Excitation E + SF6 → E + SF6(3v1) (E = 0.288096 eV, complete set) | Updated: 23 February 2016.
6. Excitation E + SF6 → E + SF6(4v1) (E = 0.384128 eV, complete set) | Updated: 23 February 2016.
7. Excitation E + SF6 → E + SF6(5v1)+higher harmonics (E = 0.48016 eV, complete set) | Updated: 23 February 2016.

Phelps database

Data Group [SF6]
e / SF6

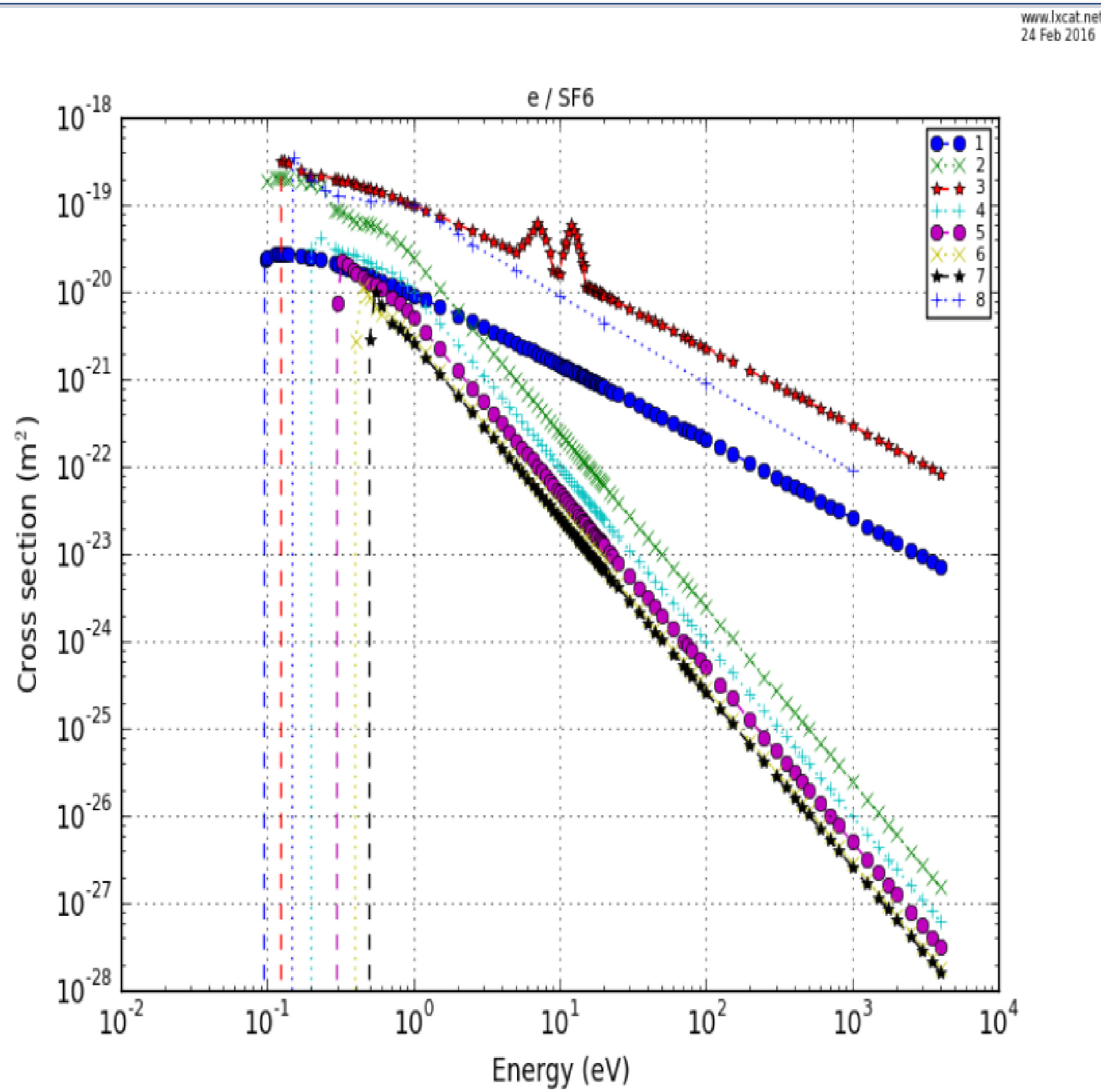
8. Excitation E + SF6 → E + SF6(0.095eV) (E = 0.095 eV, complete set) | VIBRATIONAL Excitation ROHR AND HAYASHI. Updated: 19 September 2009.

LXCAT web site

SF6 vibrations

Cross section

GO BACK | KEEP WINDOW AND GO BACK | RESCALE IN NEW WINDOW | DOWNLOAD: TXT | PNG | XML | ZIP



Biagi-v8.3 (Compilation of electron cross sections used by S.F. Biagi)

Data Group [Mbltz version 10.6]
e / SF6

1. Excitation E + SF6 → E + SF6(v4) (E = 0.076253 eV, complete set) | anisotropic. Updated: 23 February 2016 18:01.
2. Excitation E + SF6 → E + SF6(V1) (E = 0.096032 eV, complete set) | Updated: 23 February 2016 18:02.
3. Excitation E + SF6 → E + SF6(v3) (E = 0.11754 eV, complete set) | anisotropic. Updated: 23 February 2016.
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5. Excitation E + SF6 → E + SF6(3v1) (E = 0.288096 eV, complete set) | Updated: 23 February 2016.
6. Excitation E + SF6 → E + SF6(4v1) (E = 0.384128 eV, complete set) | Updated: 23 February 2016.
7. Excitation E + SF6 → E + SF6(5v1)+higher harmonics (E = 0.48016 eV, complete set) | Updated: 23 February 2016.

Phelps database

Data Group [SF6]
e / SF6

8. Excitation E + SF6 → E + SF6(0.095eV) (E = 0.095 eV, complete set) | VIBRATIONAL Excitation ROHR AND HAYASHI. Updated: 19 September 2009.

LXCAT web site SF6 excitation from 9.6 to 11.7 ev

Cross section

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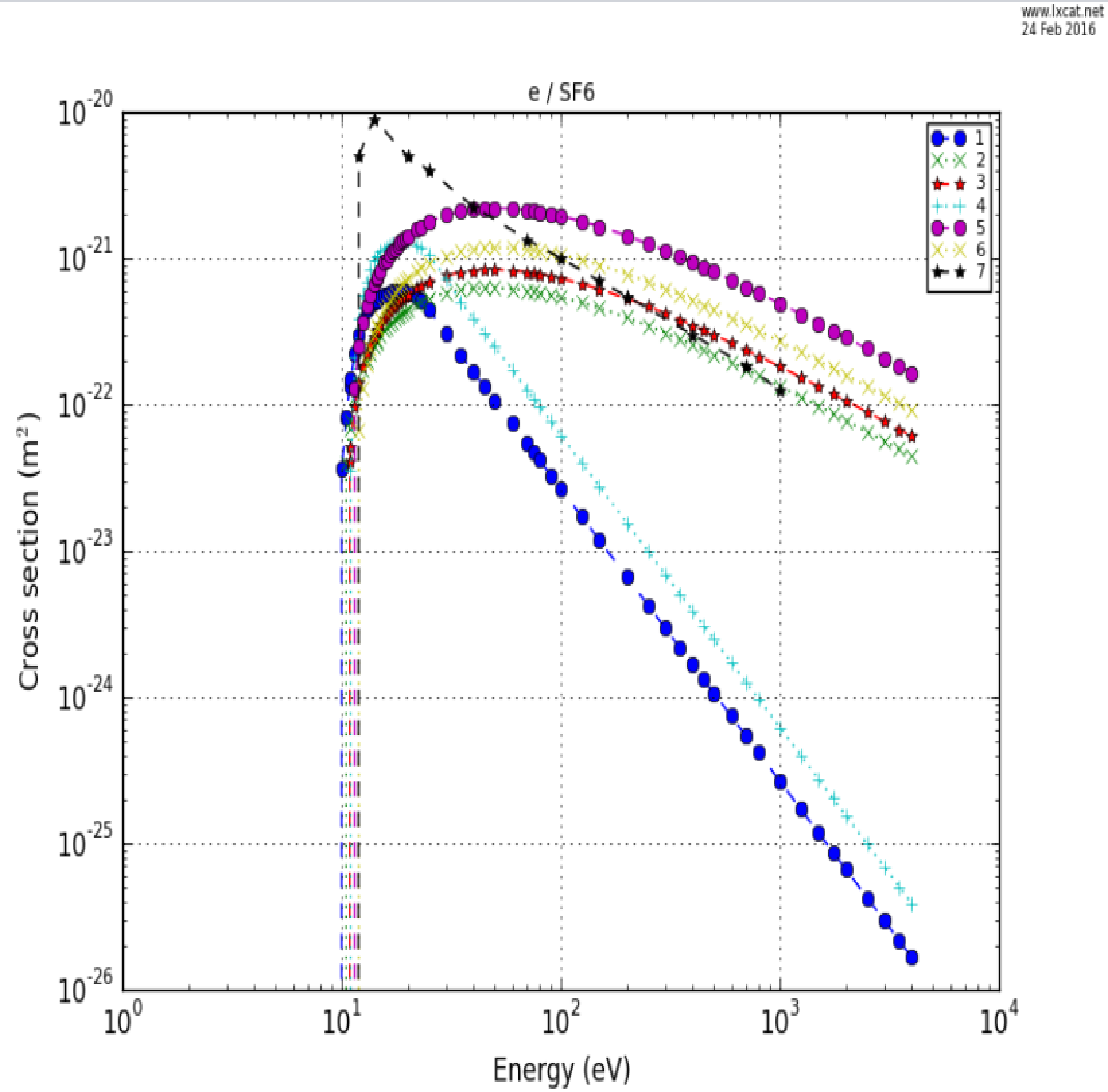

Biagi-v8.3 (Compilation of electron cross sections used by S.F. Biagi)

Data Group [Mbltz version 10.6]

e / SF6

1. Excitation E + SF6 → E + EXC. TRIPLET DISSOCIATION (E = 9.6 eV, complete set) | Updated: 23 February 2016.
2. Excitation E + SF6 → E + EXC. SINGLET DISSOC. F=0.0443 (E = 10 eV, complete set) | Updated: 23 February 2016.
3. Excitation E + SF6 → E + EXC. SINGLET DISSOC. F=0.0642 (E = 10.5 eV, complete set) | Updated: 23 February 2016.
4. Excitation E + SF6 → E + EXC. TRIPLET DISSOCIATION (E = 10.9 eV, complete set) | Updated: 23 February 2016.
5. Excitation E + SF6 → E + EXC. SINGLET DISSOC. F=0.1839 (E = 11 eV, complete set) | Updated: 23 February 2016.
6. Excitation E + SF6 → E + EXC. SINGLET DISSOC. F=0.1073 (E = 11.5 eV, complete set) | Updated: 23 February 2016.

Phelps database

Data Group [SF6]

e / SF6

7. Excitation E + SF6 → E + SF6(10.0eV) (E = 10 eV, complete set) | ELECTRONIC Excitation FROM HAYASHI. Updated: 2 March 2010.

LXCAT web site SF6 excitation 11.5 to 14.5 ev

Cross section

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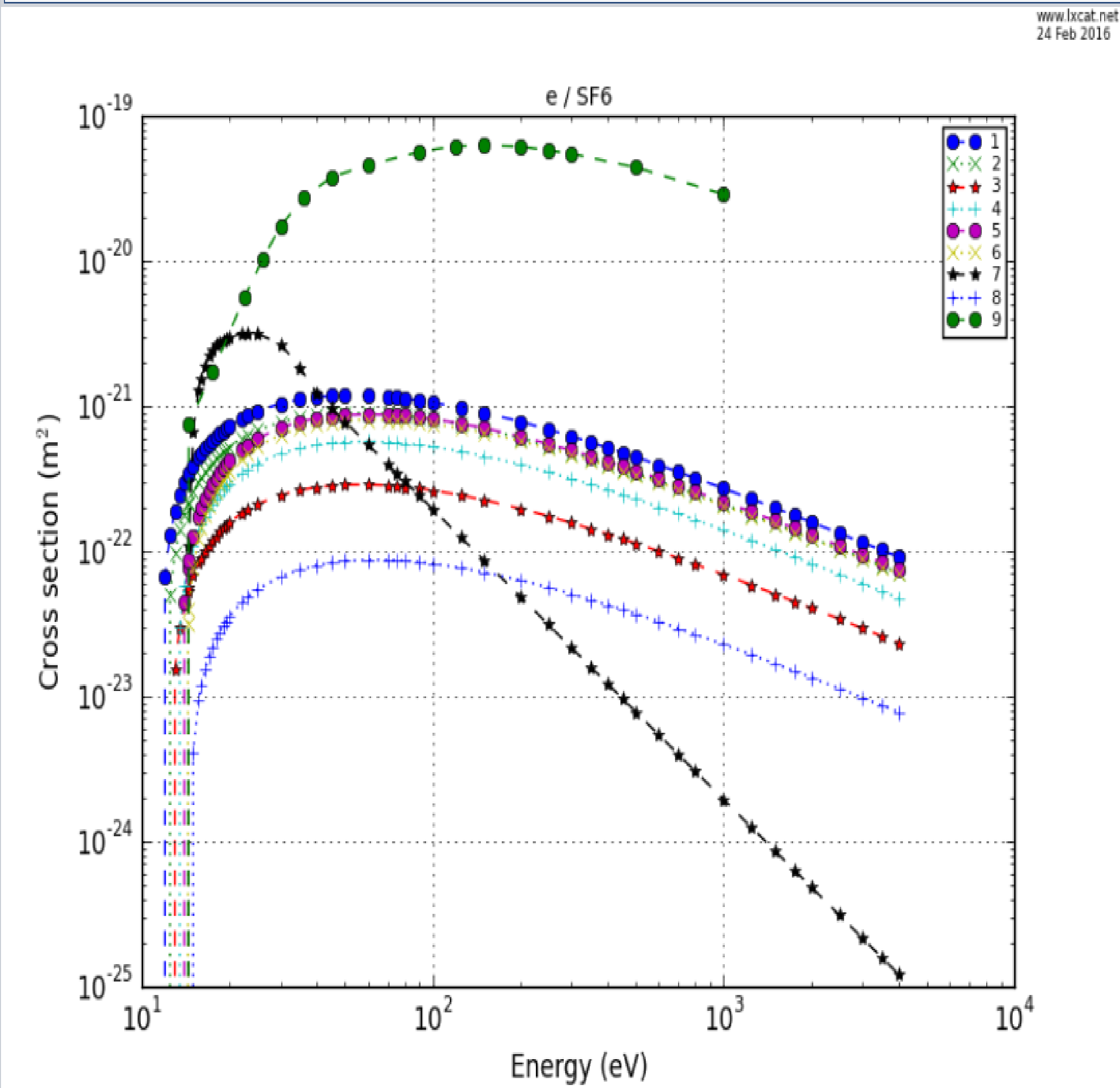


Biagi-v8.3 (Compilation of electron cross sections used by S.F. Biagi)

Data Group [Mbltz version 10.6]

e / SF6

1. Excitation E + SF6 → E + EXC. SINGLET DISSOC. F=0.1073 (E = 11.5 eV, complete set) | Updated: 23 February 2016.

2. Excitation E + SF6 → E + EXC. SINGLET DISSOC. F=0.0880 (E = 12 eV, complete set) | Updated: 23 February 2016.

3. Excitation E + SF6 → E + EXC. SINGLET DISSOC. F=0.0304 (E = 12.5 eV, complete set) | Updated: 23 February 2016.

4. Excitation E + SF6 → E + EXC. ION PAIR F- + SF5+ (E = 13 eV, complete set) | Updated: 23 February 2016.

5. Excitation E + SF6 → E + EXC. SINGLET DISSOC. F=0.1067 (E = 13.5 eV, complete set) | Updated: 23 February 2016.

6. Excitation E + SF6 → E + EXC. SINGLET DISSOC. F=0.1047 (E = 14 eV, complete set) | Updated: 23 February 2016.

7. Excitation E + SF6 → E + EXC. TRIPLET DISSOCIATION (E = 14.4 eV, complete set) | Updated: 23 February 2016.

8. Excitation E + SF6 → E + EXC. SINGLET DISSOC. F=0.1211 (E = 14.5 eV, complete set) | Updated: 23 February 2016.

Phelps database

Data Group [SF6]

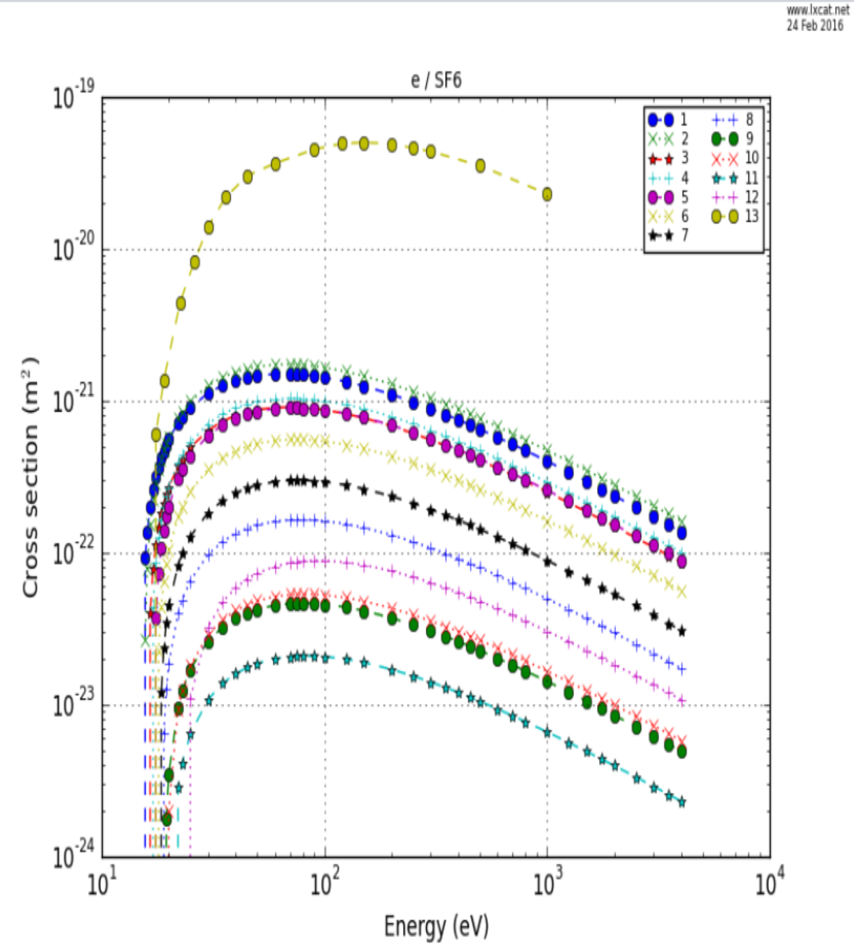
e / SF6

9. Excitation E + SF6 → E + SF6(11.7eV) (E = 11.7 eV, complete set) | Excitation - ALLOWED TRANSITION - SIMPSON,HITCHCOCK. Updated: 2 March 2010.

LXCAT web site SF6 excitation 15 to 23 ev

Cross section

GO BACK | KEEP WINDOW AND GO BACK | RESCALE IN NEW WINDOW | DOWNLOAD: TXT | PNG | XML | ZIP



Biagi-v8.3 (Compilation of electron cross sections used by S.F. Biagi)

Data Group [Mbltz version 10.6]

e / SF6

1. Excitation E + SF6 → E + EXC. SINGLET DISSOC. F=0.2225 (E = 15 eV, complete set) | Updated: 23 February 2016.
2. Excitation E + SF6 → E + EXC. SINGLET DISSOC. F=0.2731 (E = 15.5 eV, complete set) | Updated: 23 February 2016.
3. Excitation E + SF6 → E + EXC. SINGLET DISSOC. F=0.1514 (E = 16 eV, complete set) | Updated: 23 February 2016.
4. Excitation E + SF6 → E + EXC. SINGLET DISSOC. F=0.1831 (E = 16.5 eV, complete set) | Updated: 23 February 2016.
5. Excitation E + SF6 → E + EXC. SINGLET DISSOC. F=0.1678 (E = 17 eV, complete set) | Updated: 23 February 2016.
6. Excitation E + SF6 → E + EXC. SINGLET DISSOC. F=0.1098 (E = 17.5 eV, complete set) | Updated: 23 February 2016.
7. Excitation E + SF6 → E + EXC. SINGLET DISSOC. F=0.0623 (E = 18 eV, complete set) | Updated: 23 February 2016.
8. Excitation E + SF6 → E + EXC. SINGLET DISSOC. F=0.0361 (E = 18.5 eV, complete set) | Updated: 23 February 2016.
9. Excitation E + SF6 → E + EXC. SINGLET DISSOC. F=0.0107 (E = 19 eV, complete set) | Updated: 23 February 2016.
10. Excitation E + SF6 → E + EXC. SINGLET DISSOC. F=0.0129 (E = 19.5 eV, complete set) | Updated: 23 February 2016.
11. Excitation E + SF6 → E + EXC. SINGLET DISSOC. F=0.0053 (E = 20 eV, complete set) | Updated: 23 February 2016.
12. Excitation E + SF6 → E + EXC. SINGLET DISSOC. F=0.0290 (E = 23 eV, complete set) | Updated: 23 February 2016.

Phelps database

Data Group [SF6]

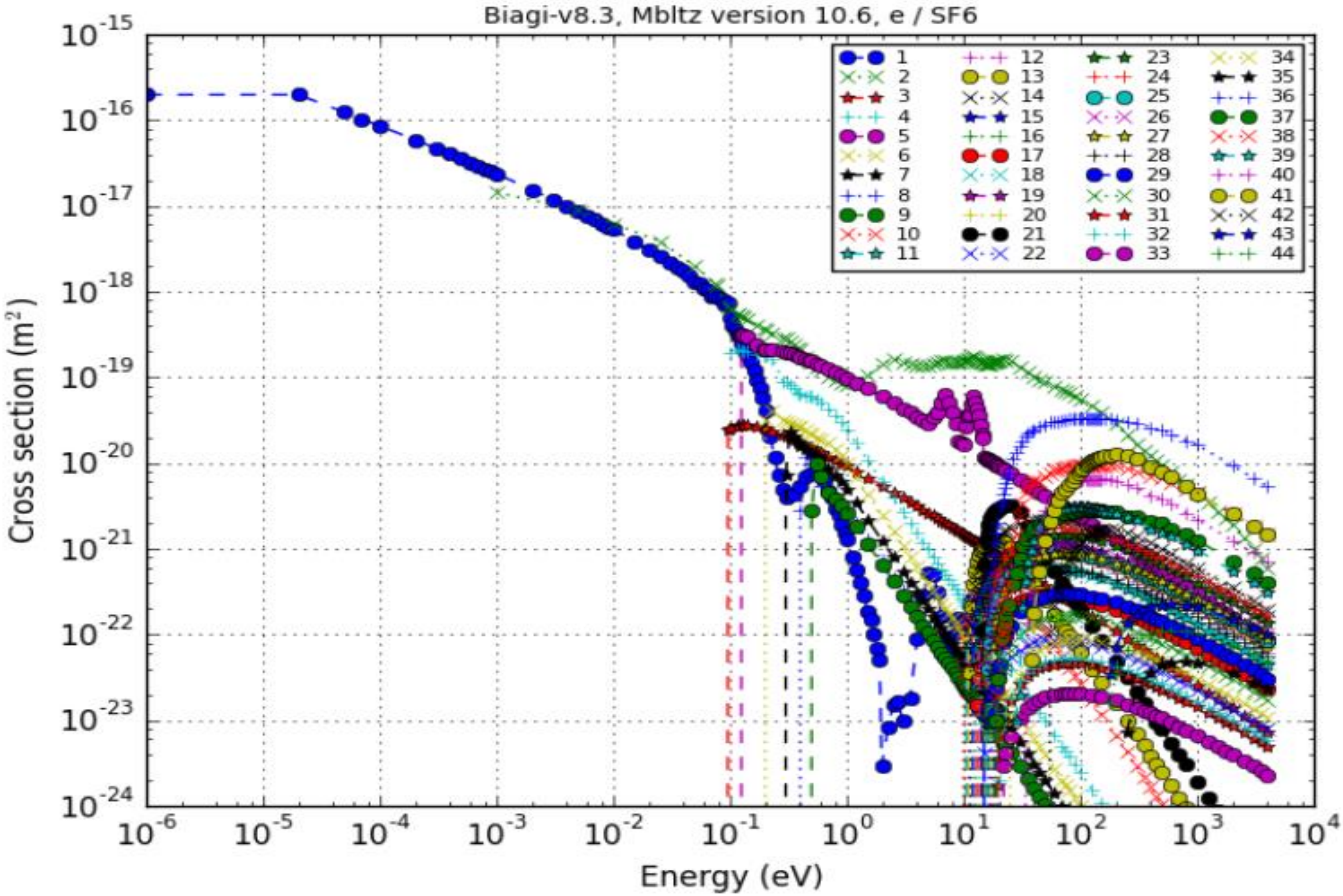
e / SF6

13. Excitation E + SF6 → E + SF6(15.0eV) (E = 15 eV, complete set) | Excitation - ALLOWED TRANSITION - SIMPSON,HITCHCOCK. Updated: 2 March 2010.

Rescale tool - Internet Explorer

http://nl.lxcat.net/data/rescale.php?id=56cc8e934024e&fig=1x6&x0=auto&x1=auto&y0=1e-24&y1=auto&REPLOT=REPLOT

www.lxcat.net
23 Feb 2016

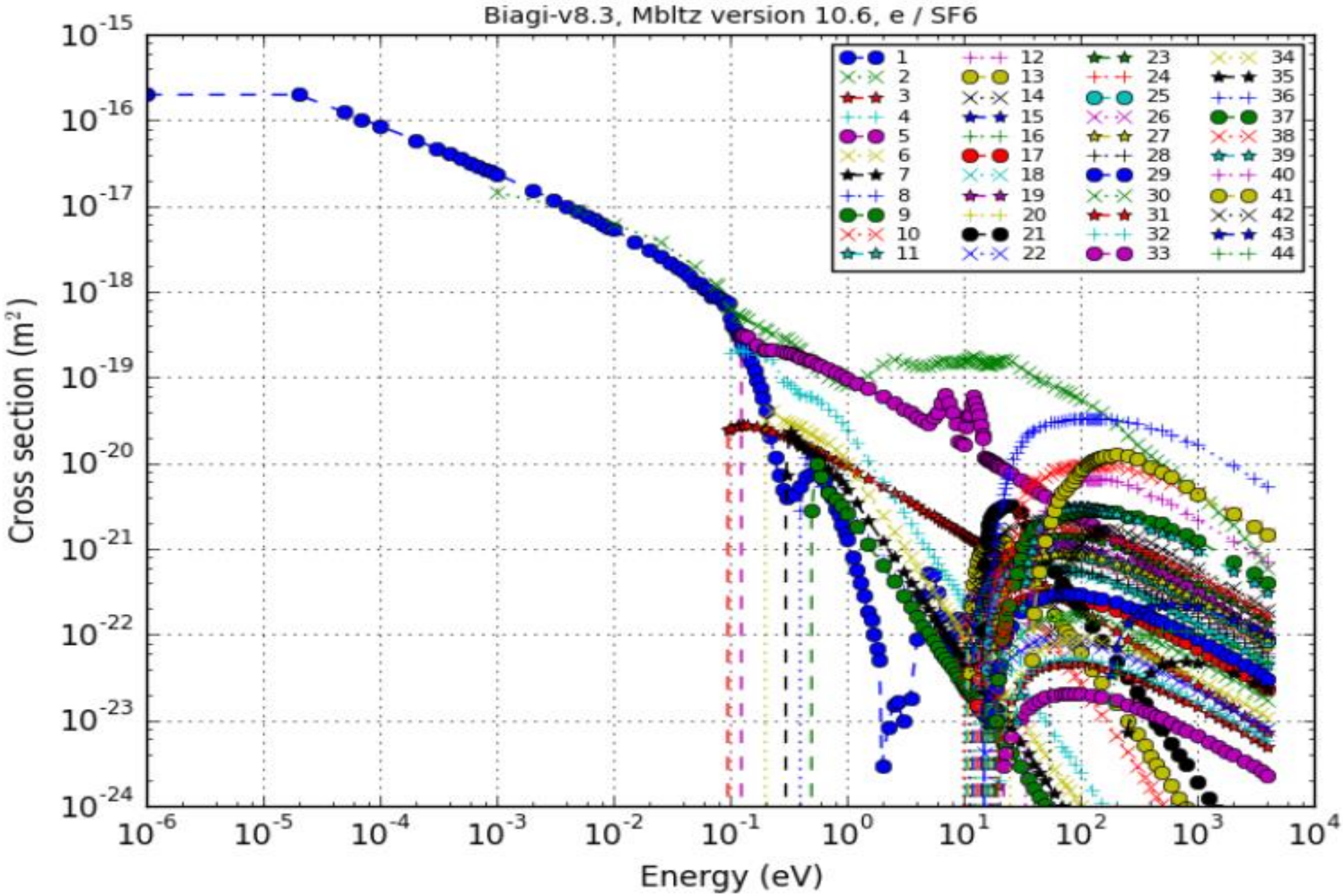


= auto — auto ○ linear ○ log REPLOT Y = 1.0E-24 — auto ○ linear ○ log

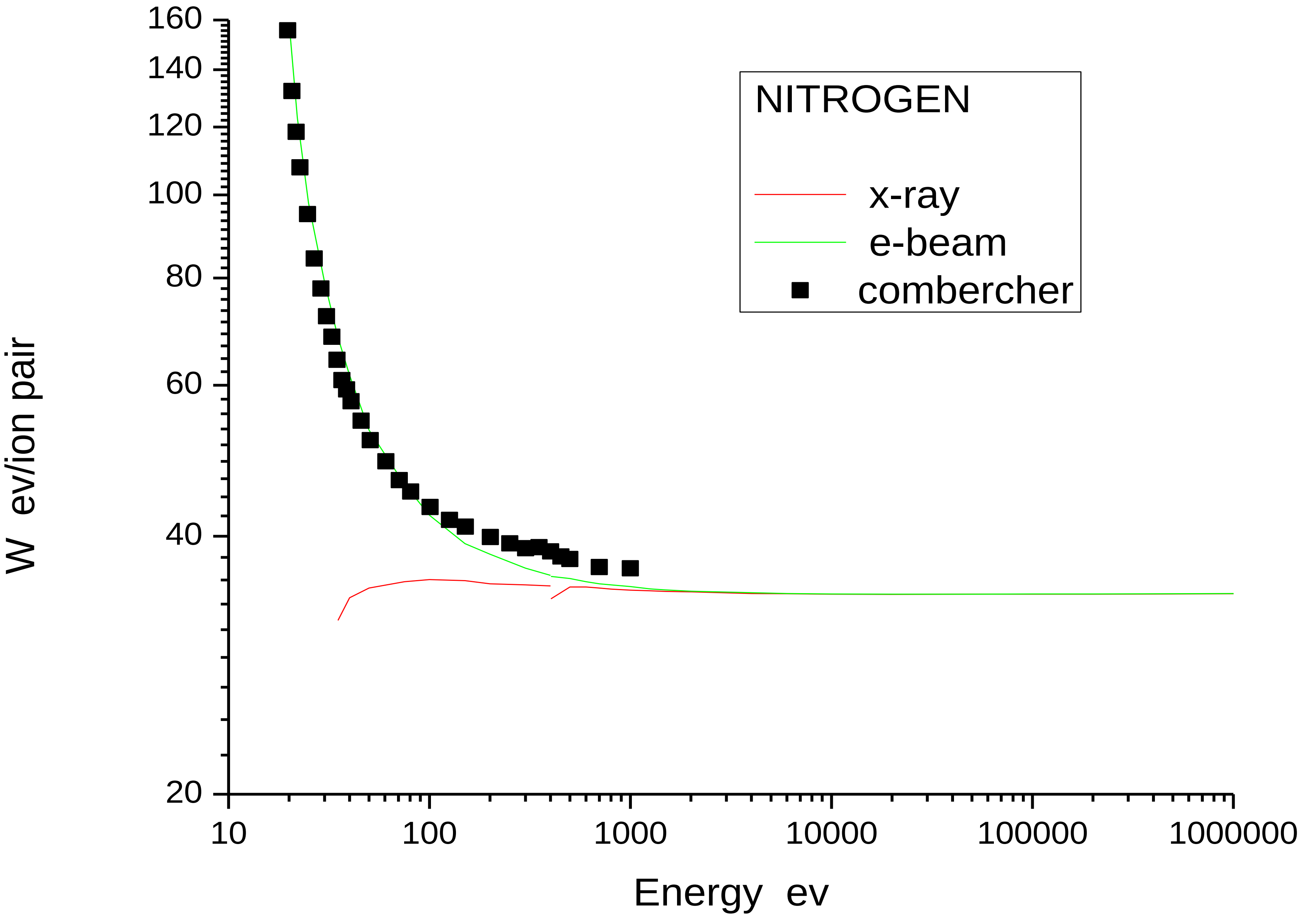
Rescale tool - Internet Explorer

http://nl.lxcat.net/data/rescale.php?id=56cc8e934024e&fig=1x6&x0=auto&x1=auto&y0=1e-24&y1=auto&REPLOT=REPLOT

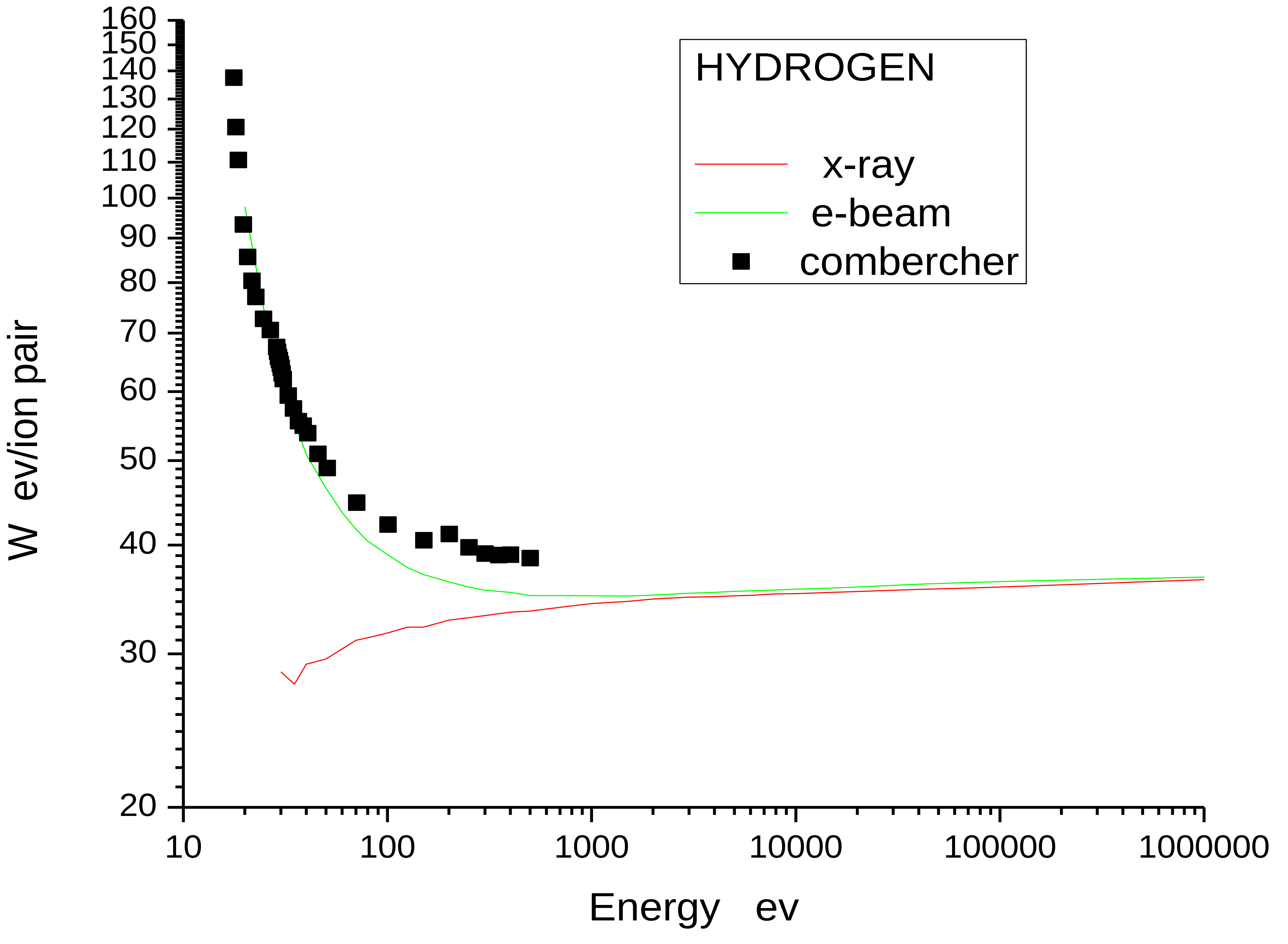
www.lxcat.net
23 Feb 2016

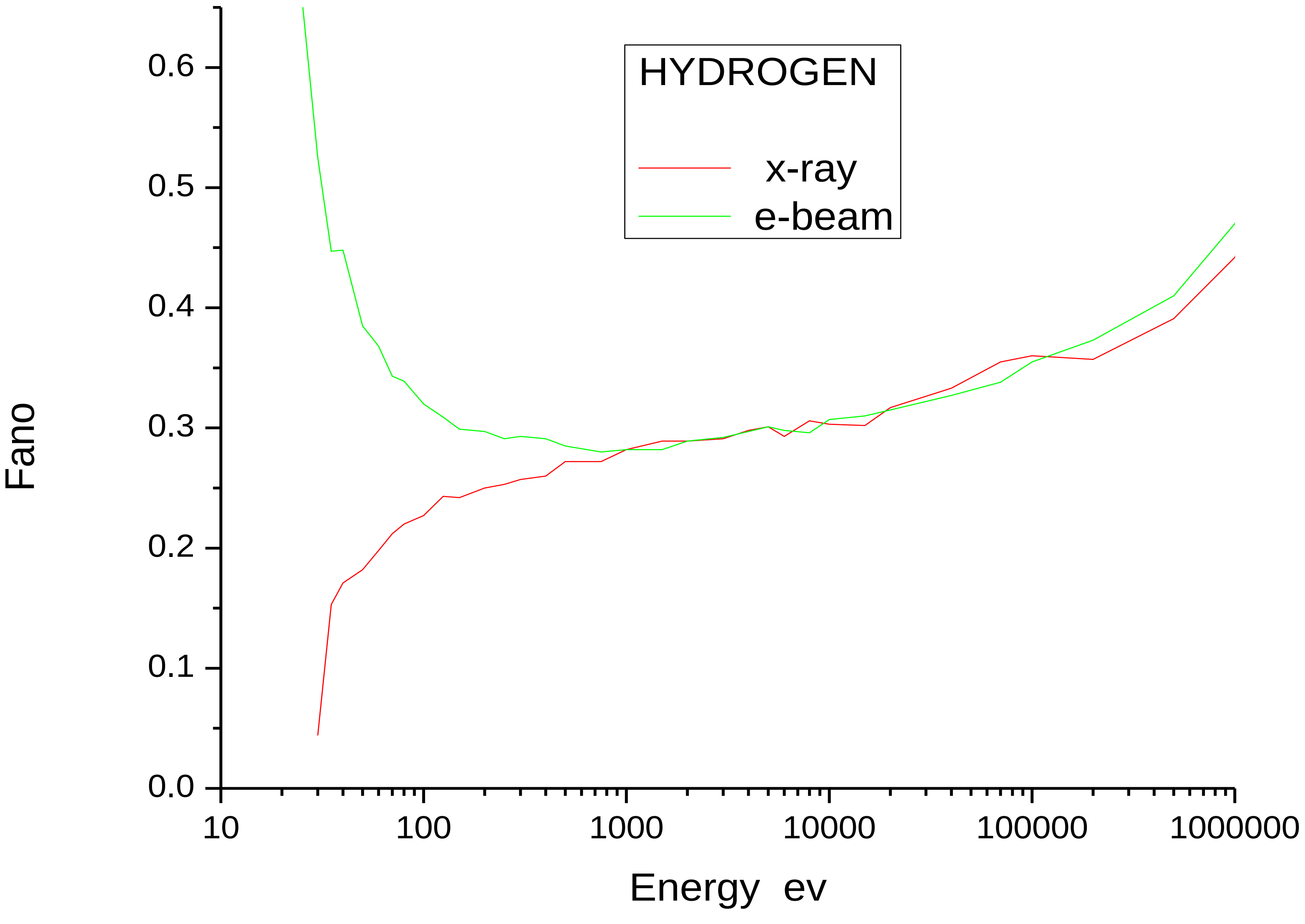


= auto — auto linear log REPLOT Y = 1.0E-24 — auto linear log

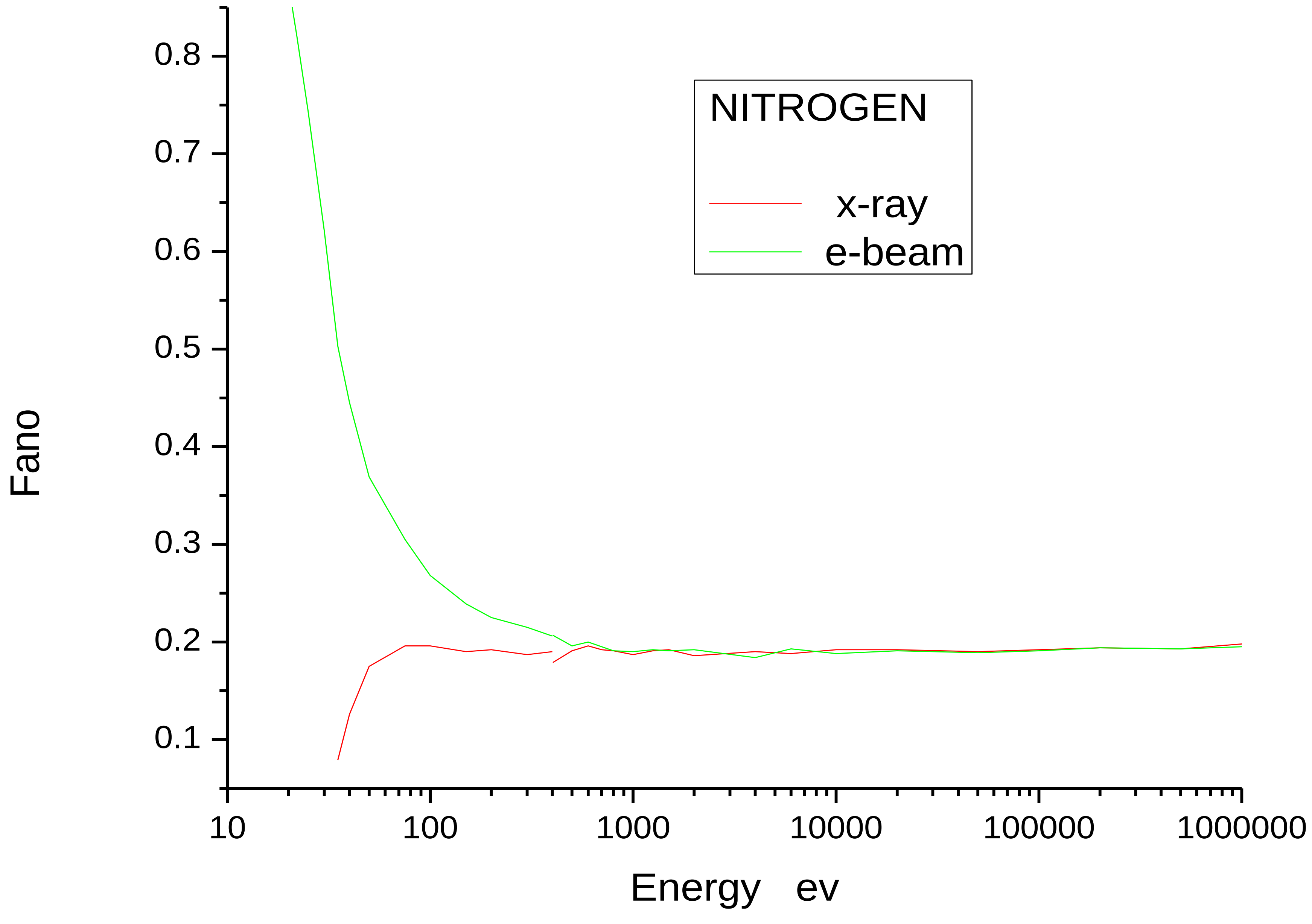


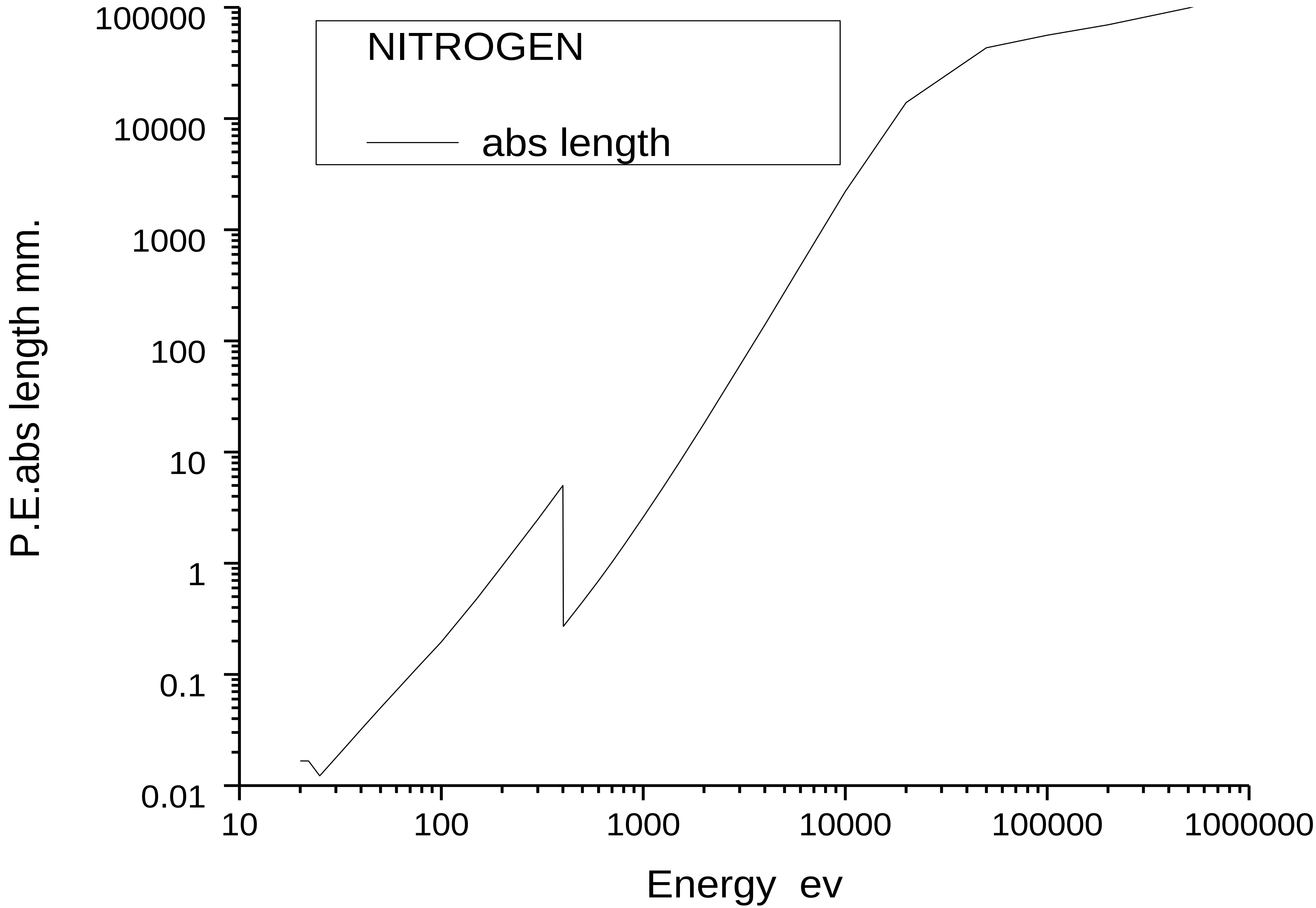
NITROGEN
x-ray
e-beam
combercher
W ev/ion pair
Energy ev
160
140
120
100
80
60
40
20
10
100
1000
10000
100000
1000000


HYDROGEN
x-ray
e-beam
combercher
W ev/ion pair
Energy ev
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
100
1000
10000
100000
1000000

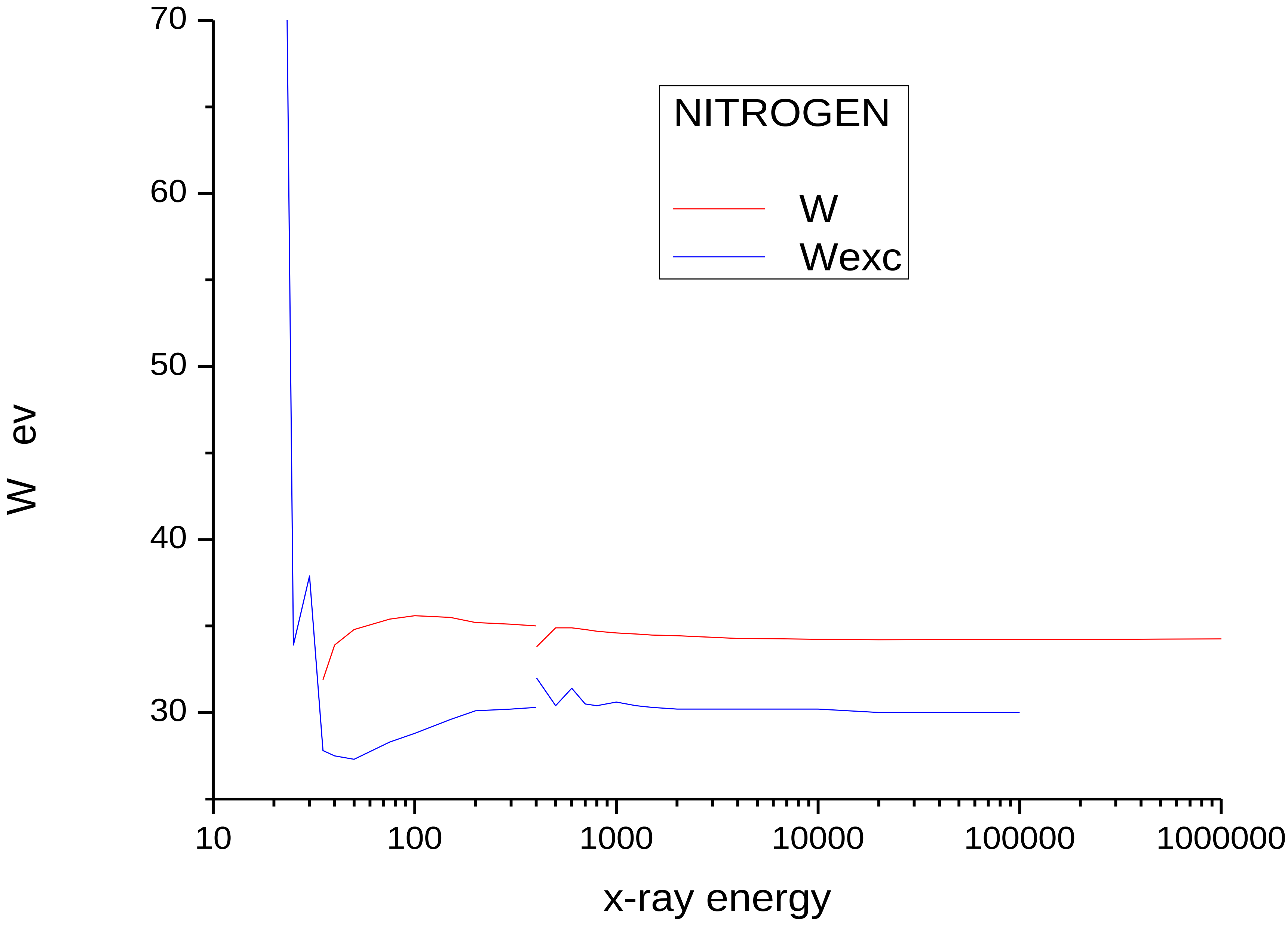


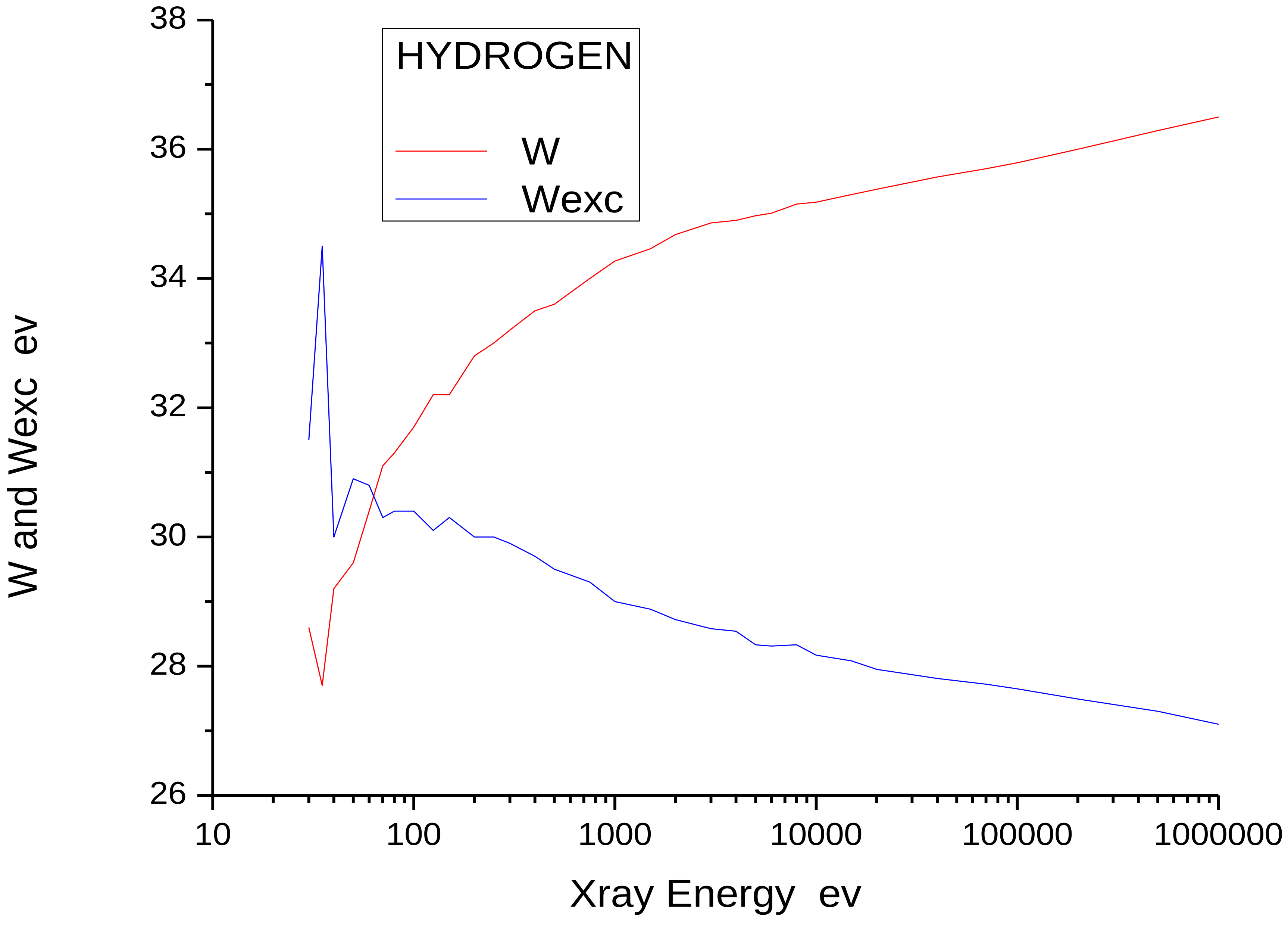
HYDROGEN
x-ray
e-beam
Fano
Energy ev
0.0
0.1
0.2
0.3
0.4
0.5
0.6
10
100
1000
10000
100000
1000000

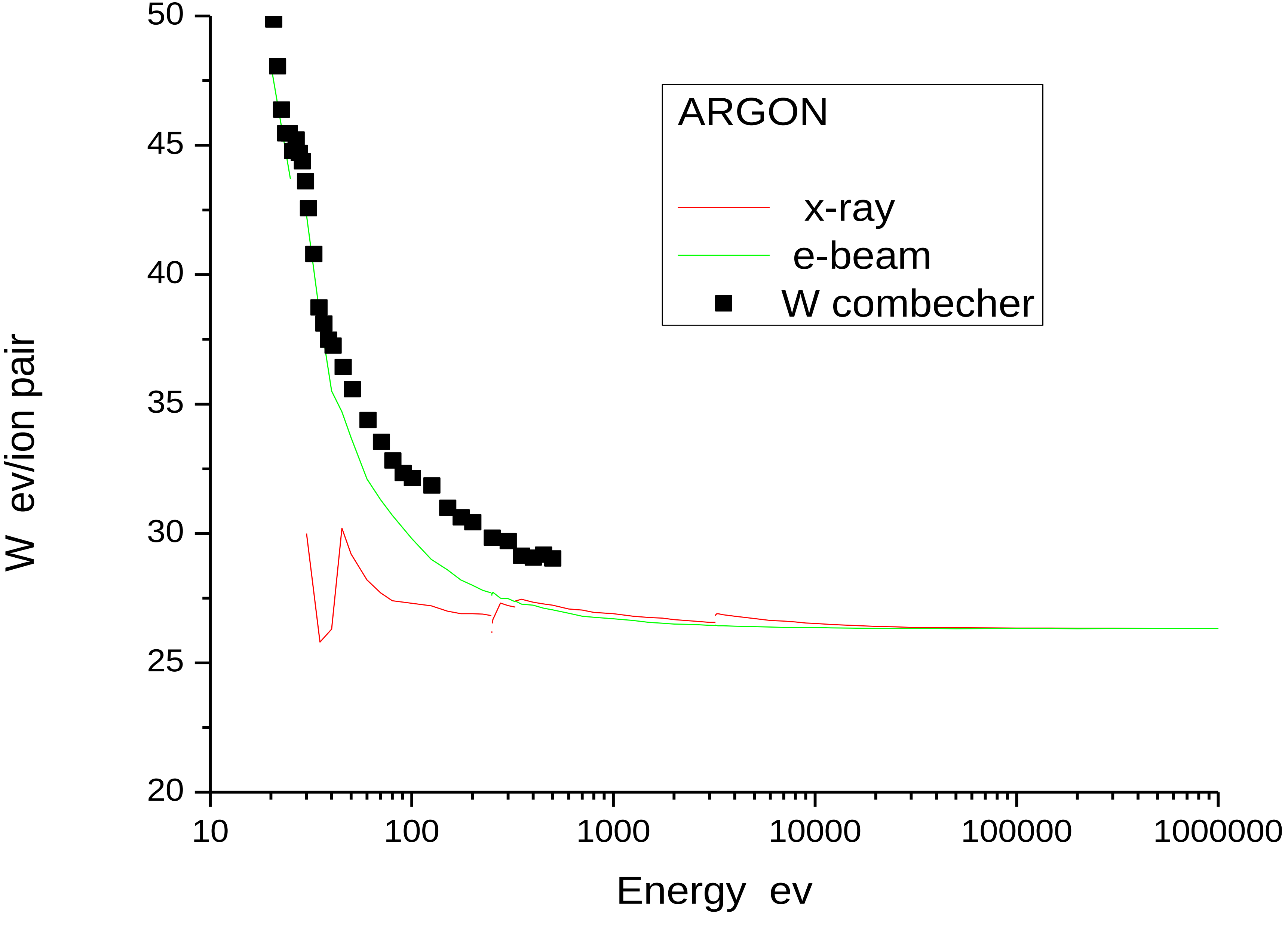

NITROGEN
x-ray
e-beam
Fano
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
10
100
1000
10000
100000
1000000
Energy ev



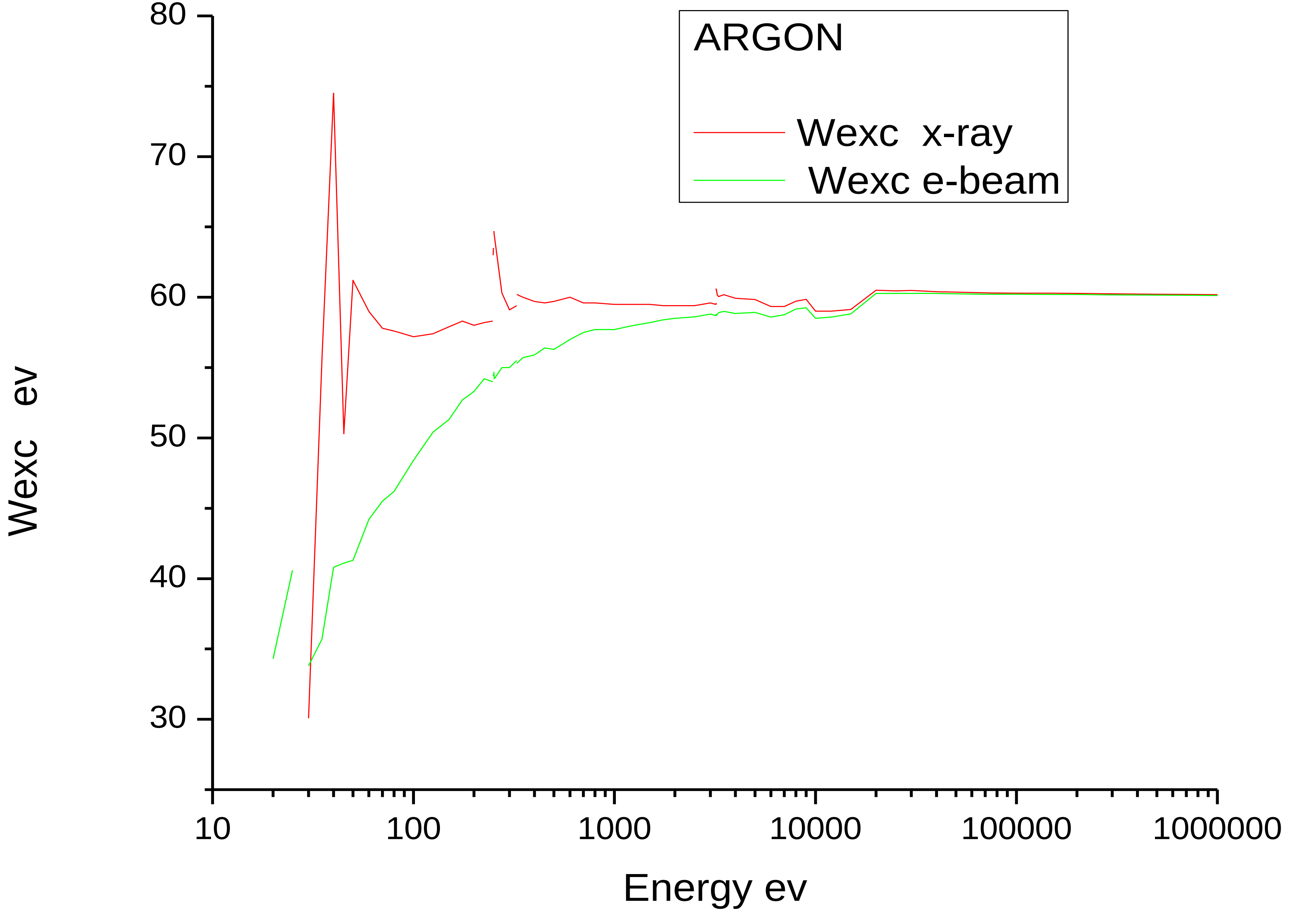
NITROGEN
abs length
P.E.abs length mm.
100000
10000
1000
100
10
1
0.1
0.01
10
100
1000
10000
100000
1000000
Energy ev


NITROGEN
W
Wexc
70
60
50
40
30
W ev
10
100
1000
10000
100000
1000000
x-ray energy

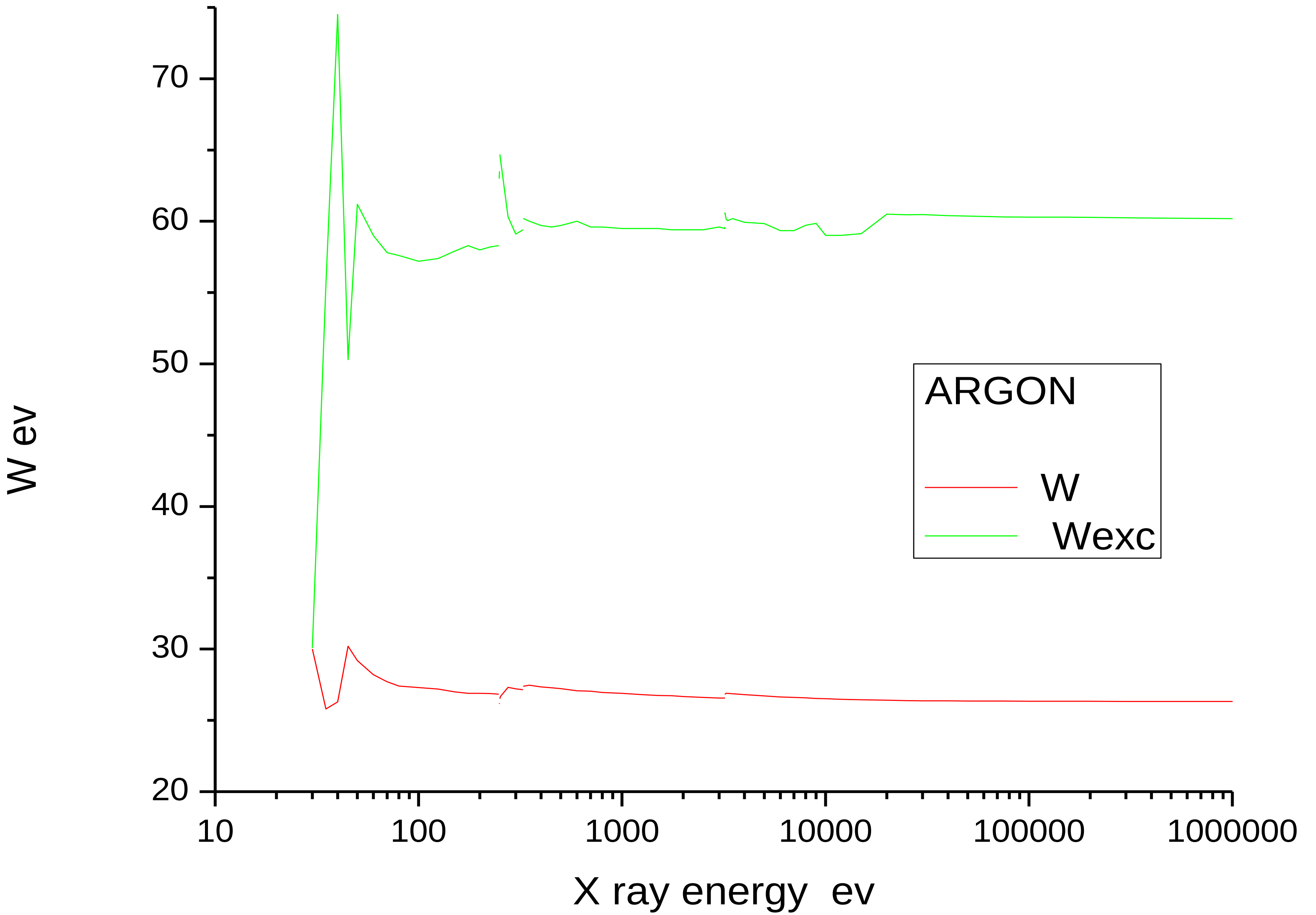

HYDROGEN
W
Wexc
W and Wexc ev
Xray Energy ev
38
36
34
32
30
28
26
10
100
1000
10000
100000
1000000



ARGON
x-ray
e-beam
W combecher
W ev/ion pair
Energy ev
50
45
40
35
30
25
20
10
100
1000
10000
100000
1000000



ARGON
Wexc x-ray
Wexc e-beam
80
70
60
50
40
30
Wexc ev
10
100
1000
10000
100000
1000000
Energy ev



ARGON
W
Wexc
W ev
X ray energy ev
70
60
50
40
30
20
10
100
1000
10000
100000
1000000

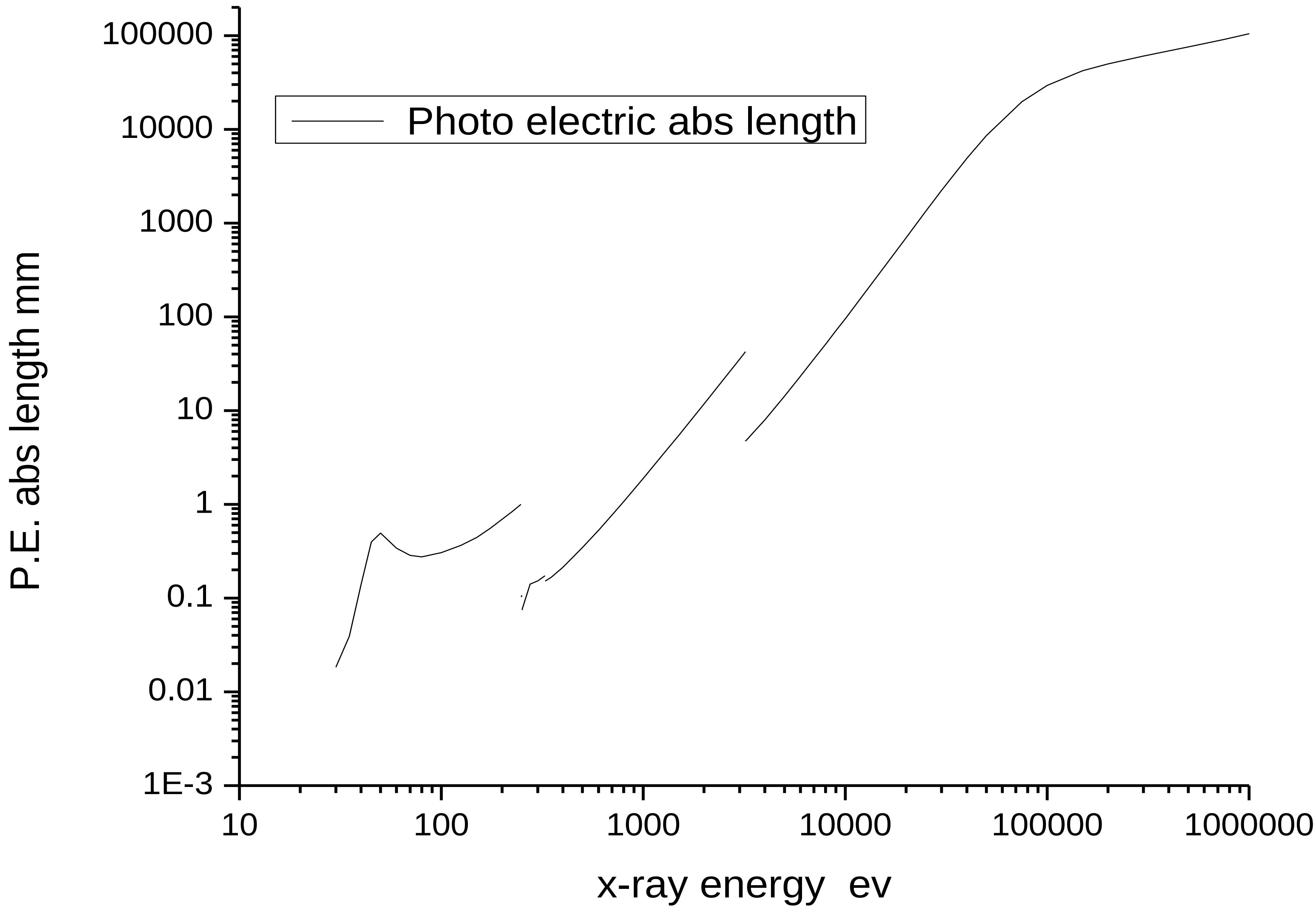
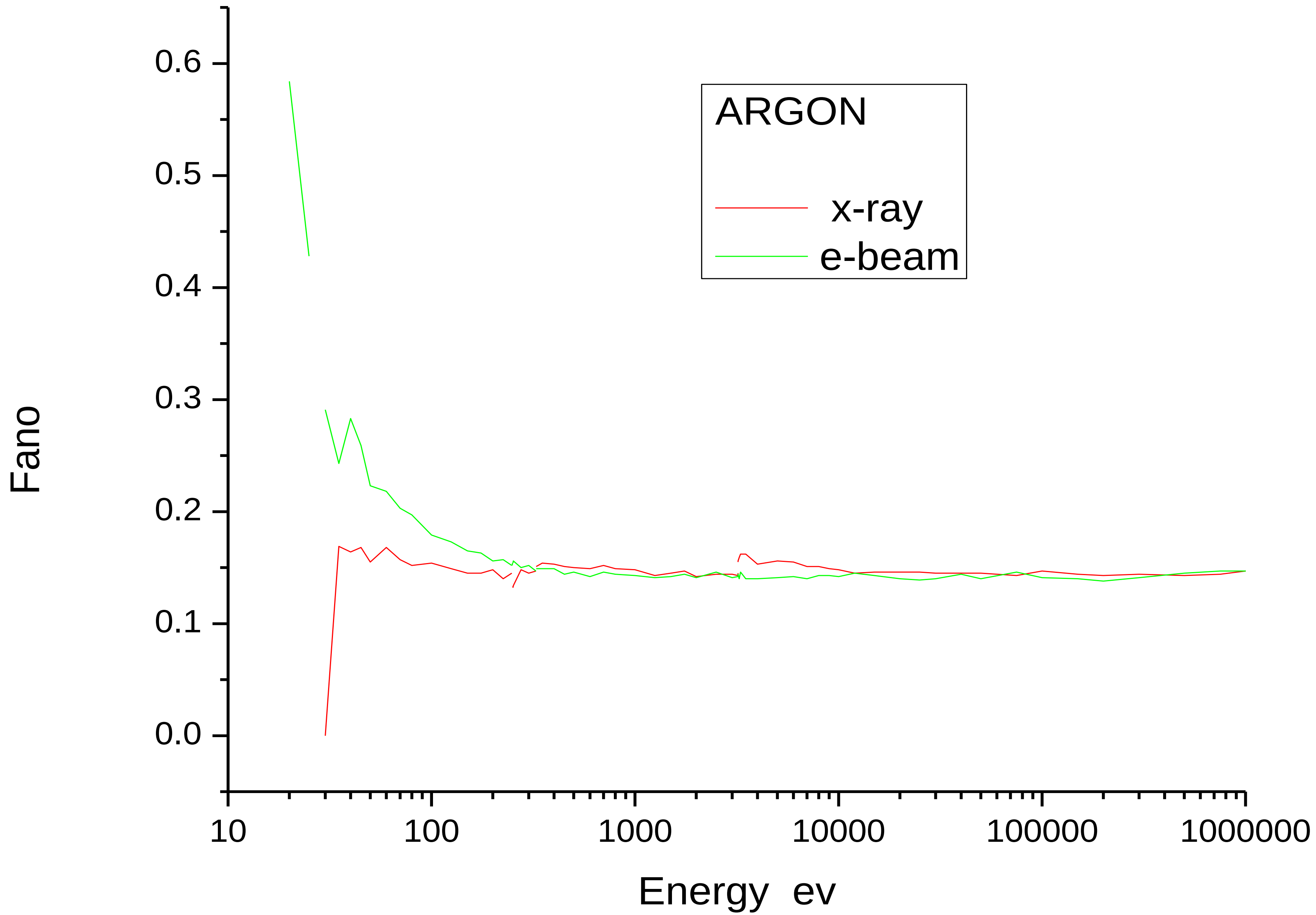
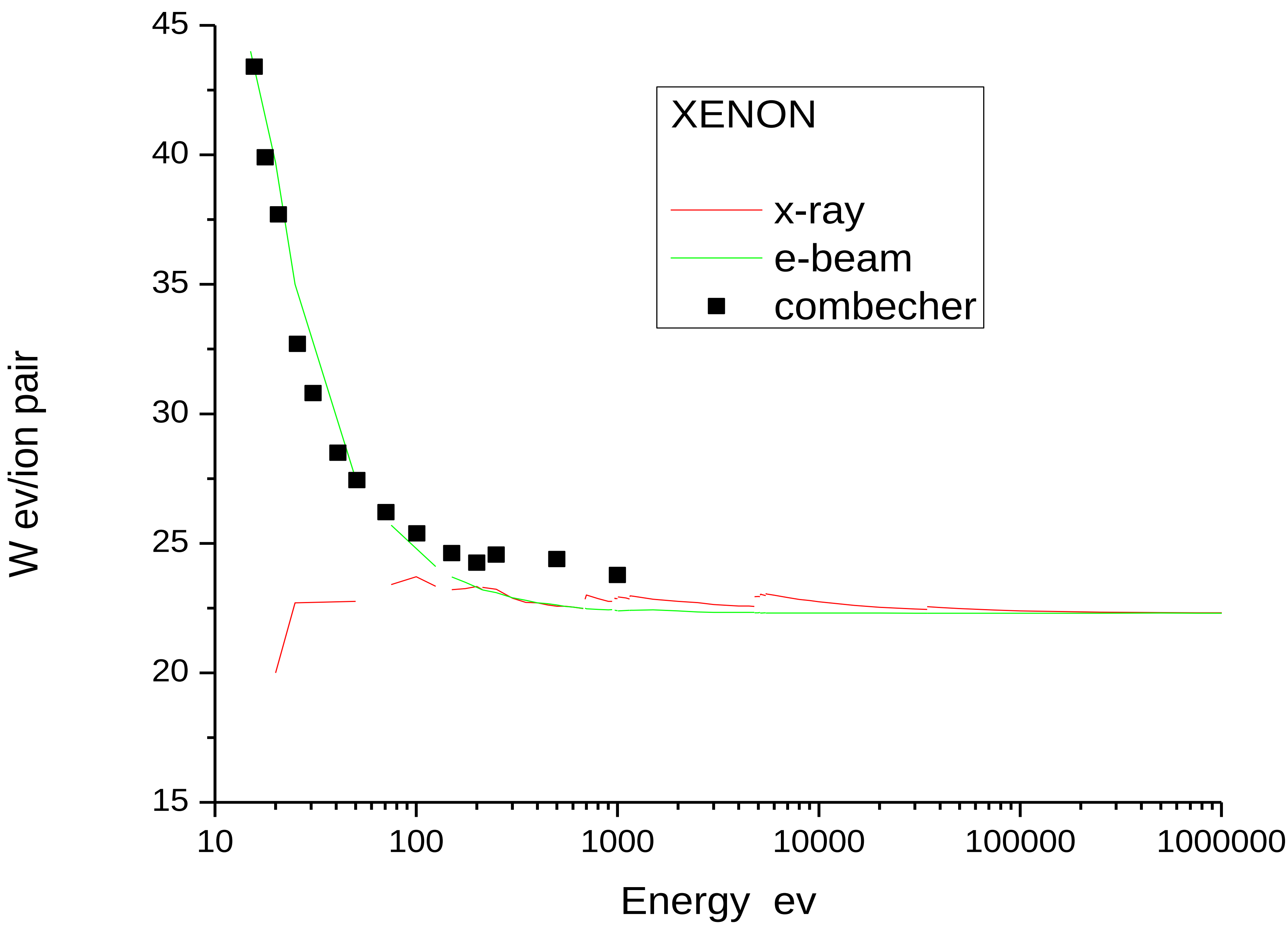


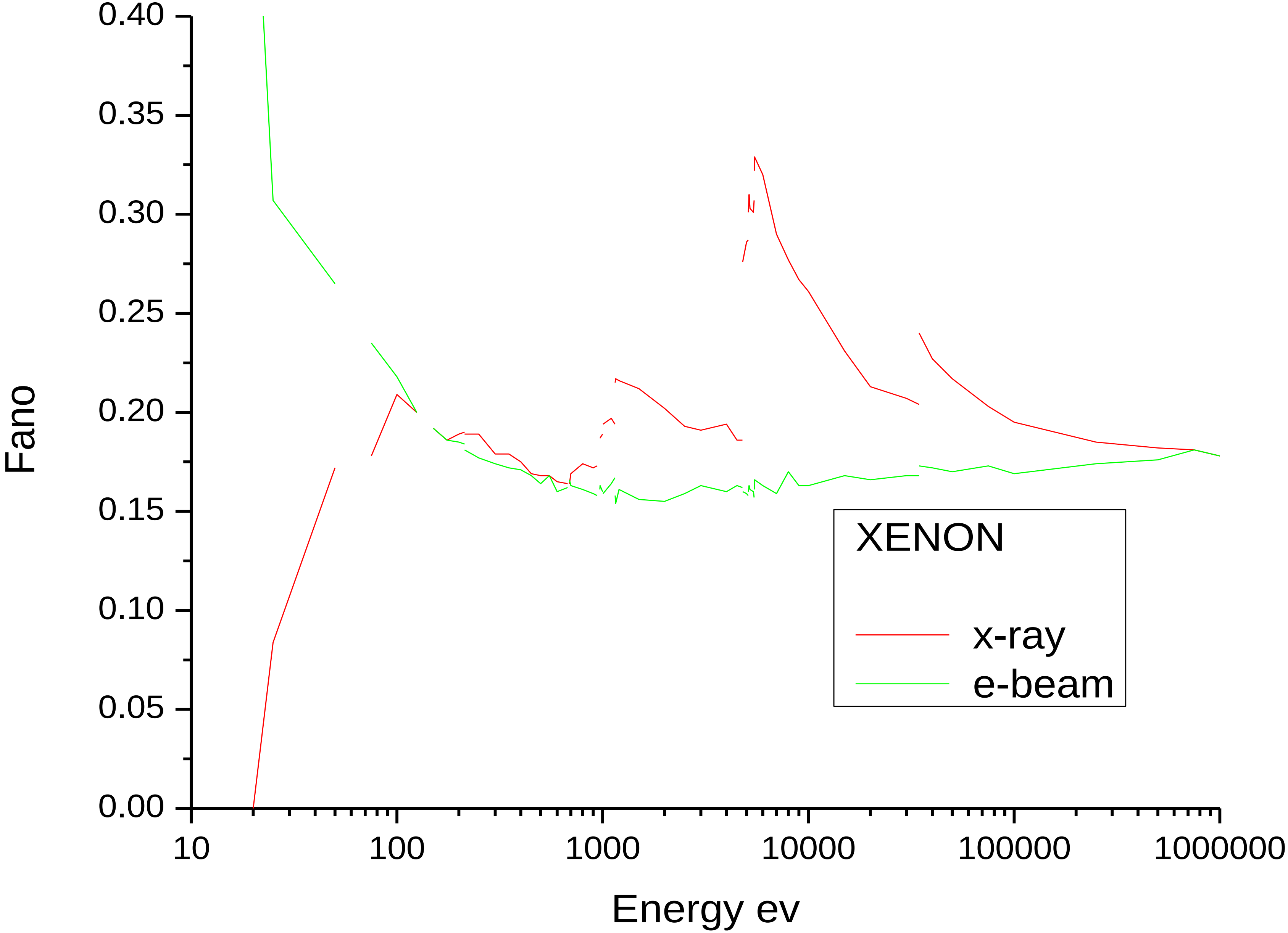
Photo electric abs length
P.E. abs length mm
100000
10000
1000
100
10
1
0.1
0.01
1E-3
10
100
1000
10000
100000
1000000
x-ray energy ev



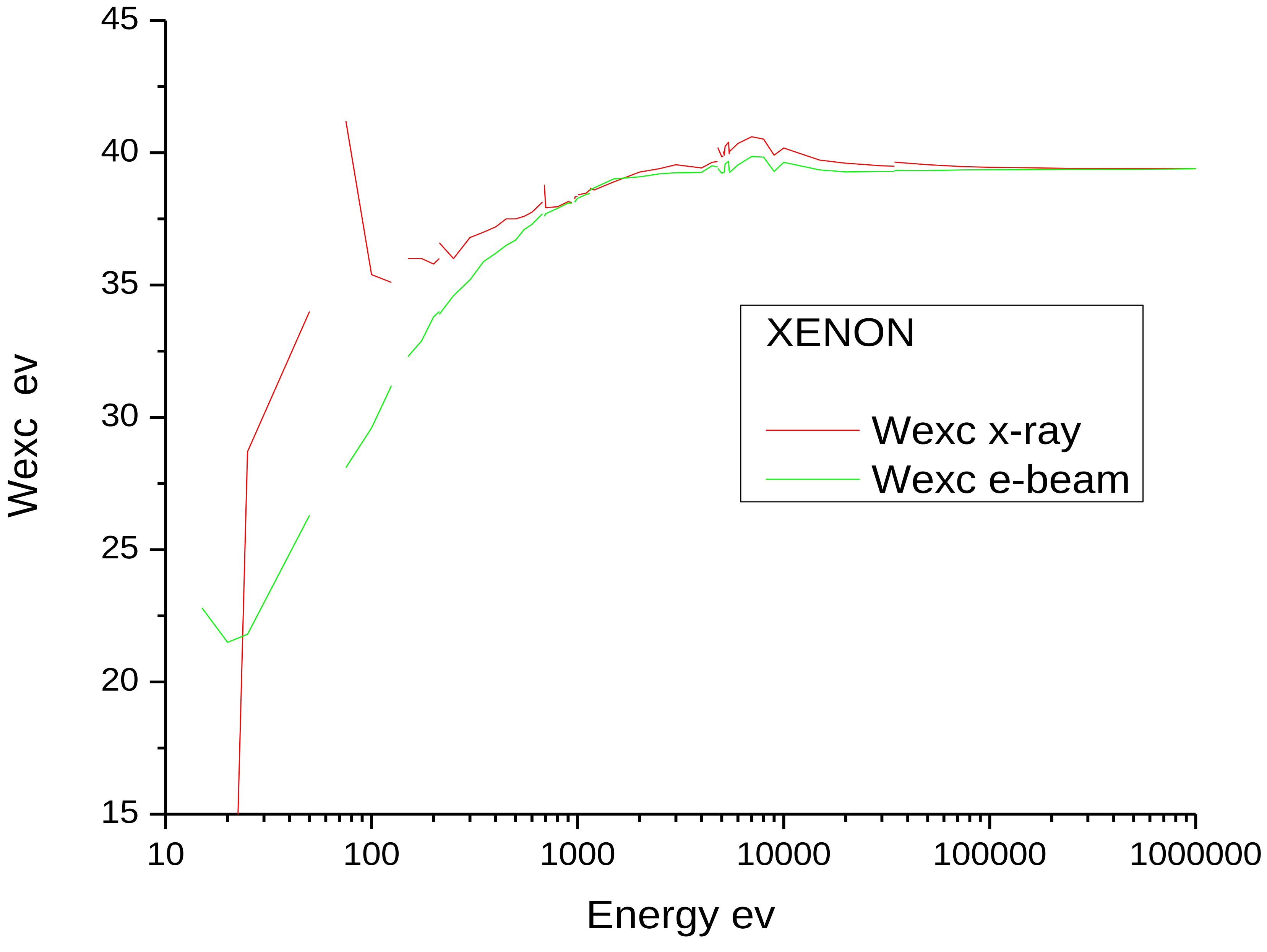
ARGON
x-ray
e-beam
Fano
0.0
0.1
0.2
0.3
0.4
0.5
0.6
10
100
1000
10000
100000
1000000
Energy ev



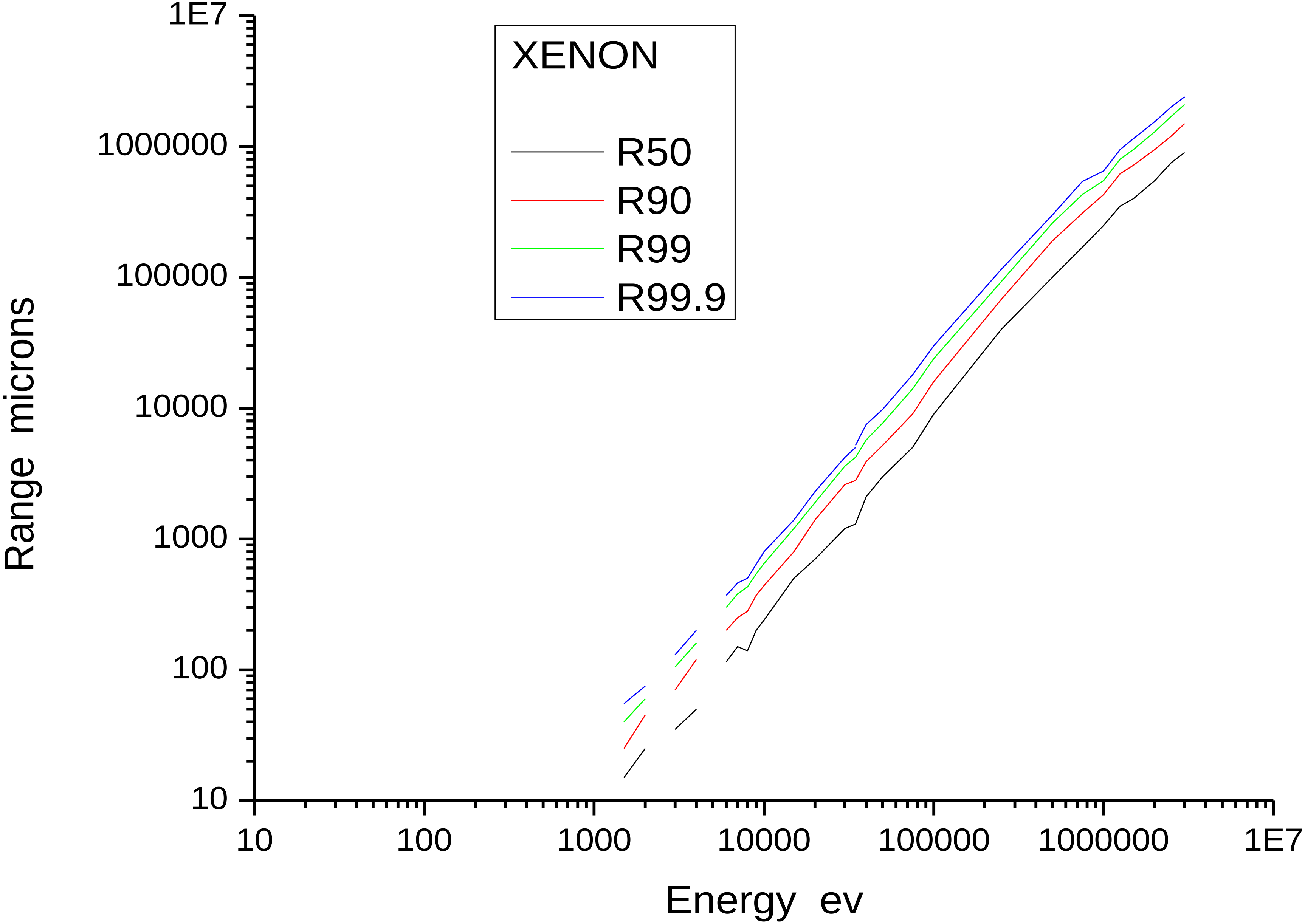
XENON
x-ray
e-beam
combecher
W ev/ion pair
Energy ev
45
40
35
30
25
20
15
10
100
1000
10000
100000
1000000

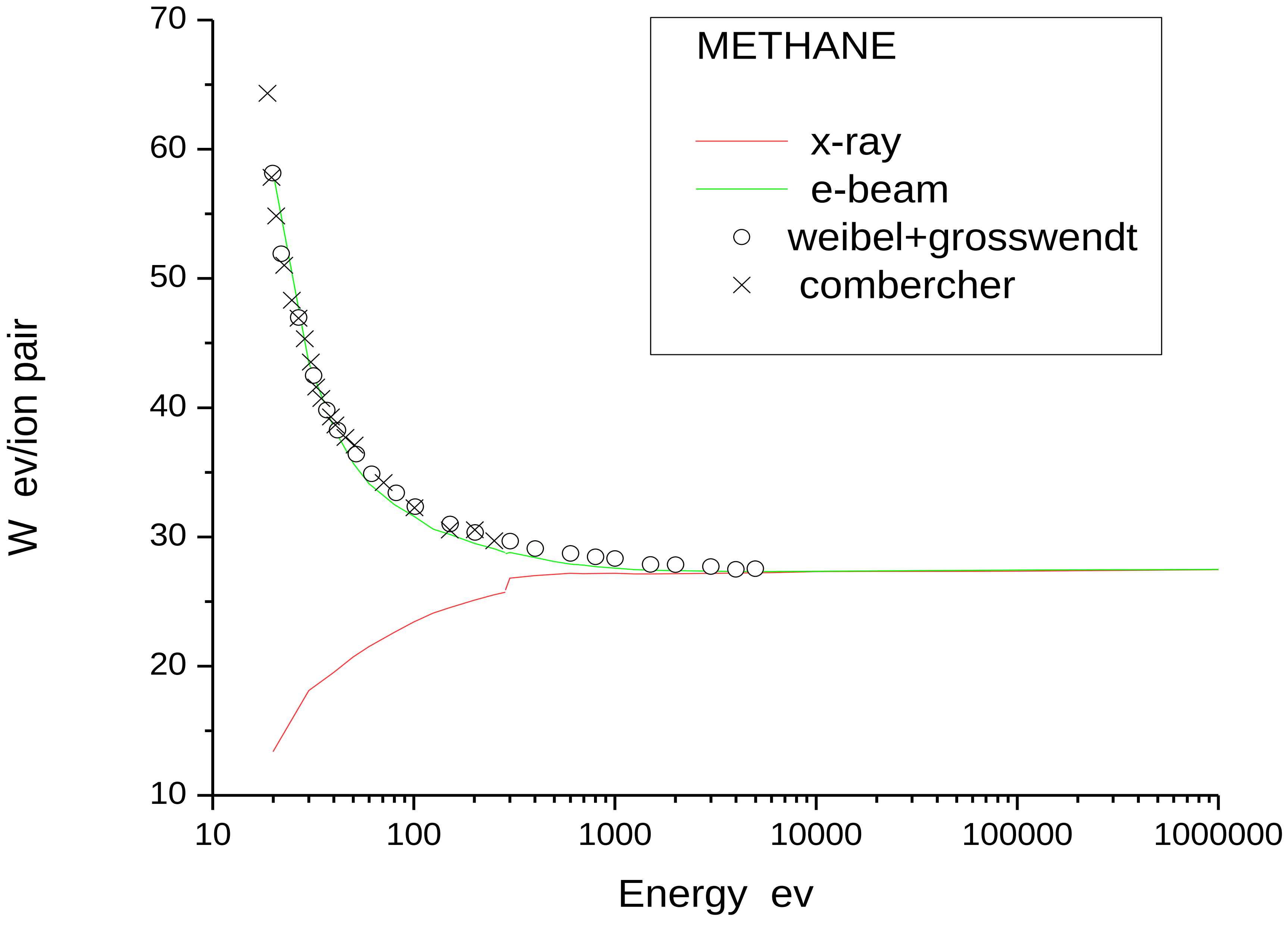


Fano
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
10
100
1000
10000
100000
1000000
Energy ev
XENON
x-ray
e-beam

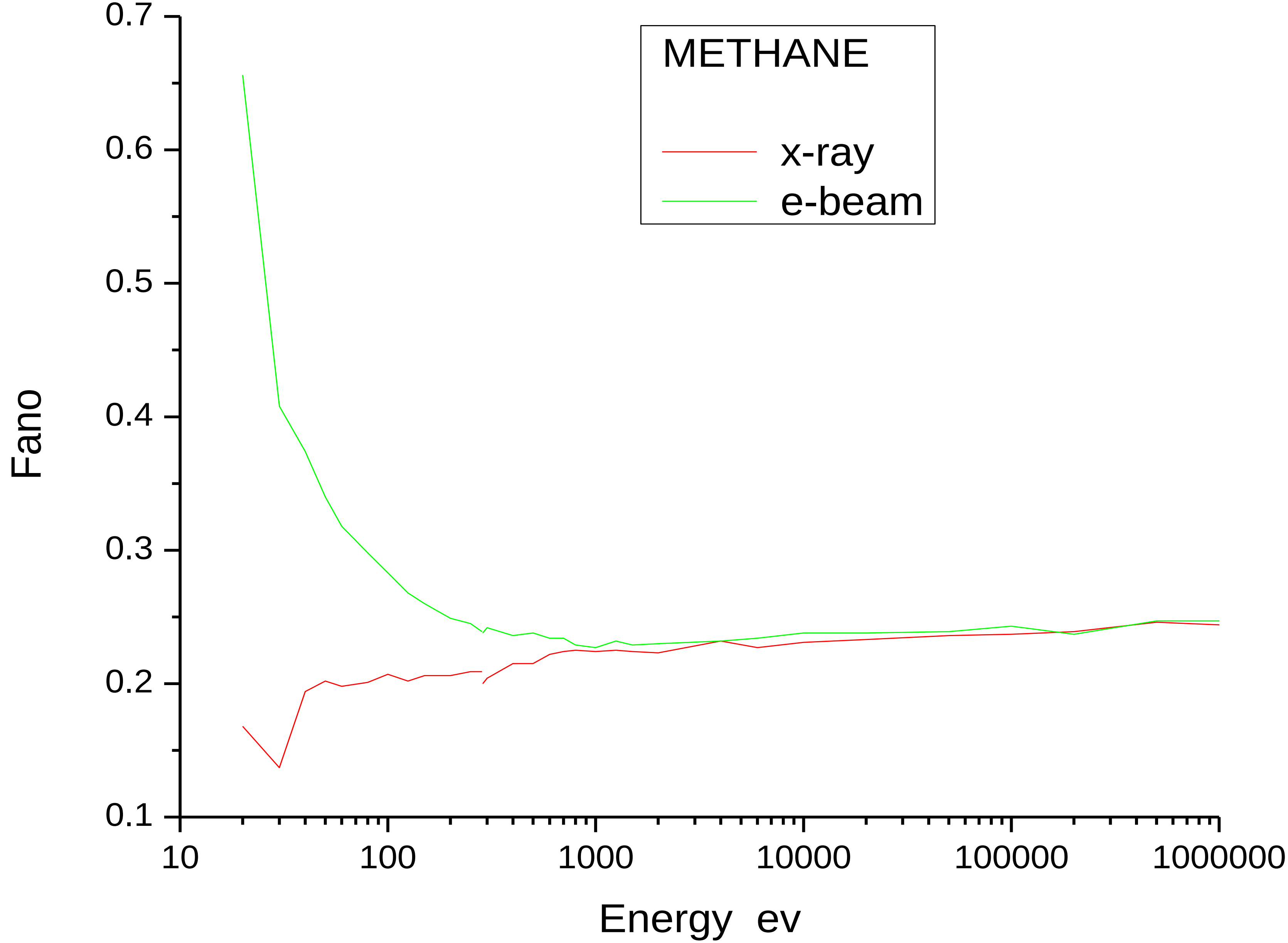


XENON
Wexc x-ray
Wexc e-beam
Wexc ev
Energy ev
45
40
35
30
25
20
15
10
100
1000
10000
100000
1000000

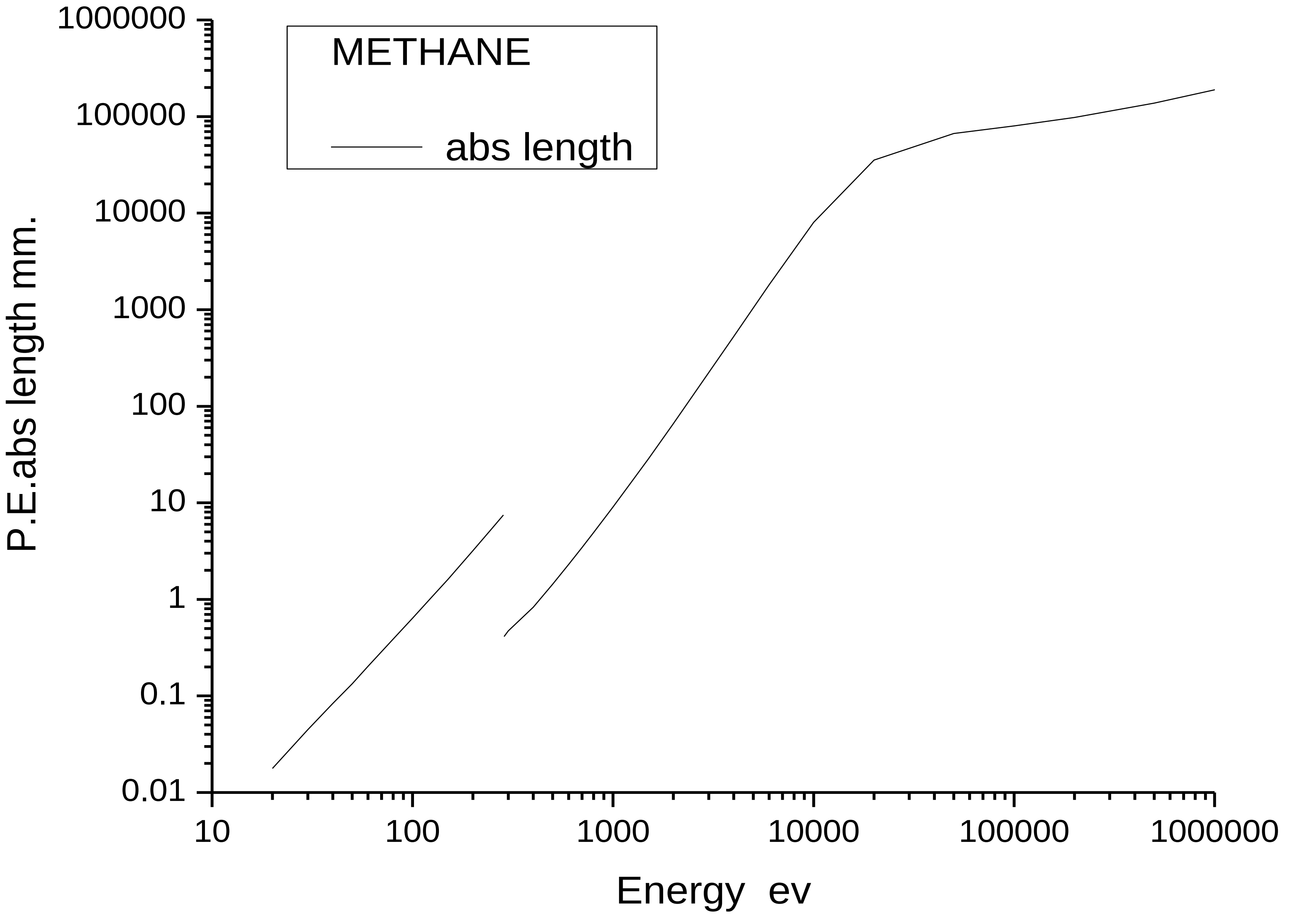

XENON
R50
R90
R99
R99.9
Range microns
Energy ev
1E7
1000000
100000
10000
1000
100
10
10
100
1000
10000
100000
1000000
1E7

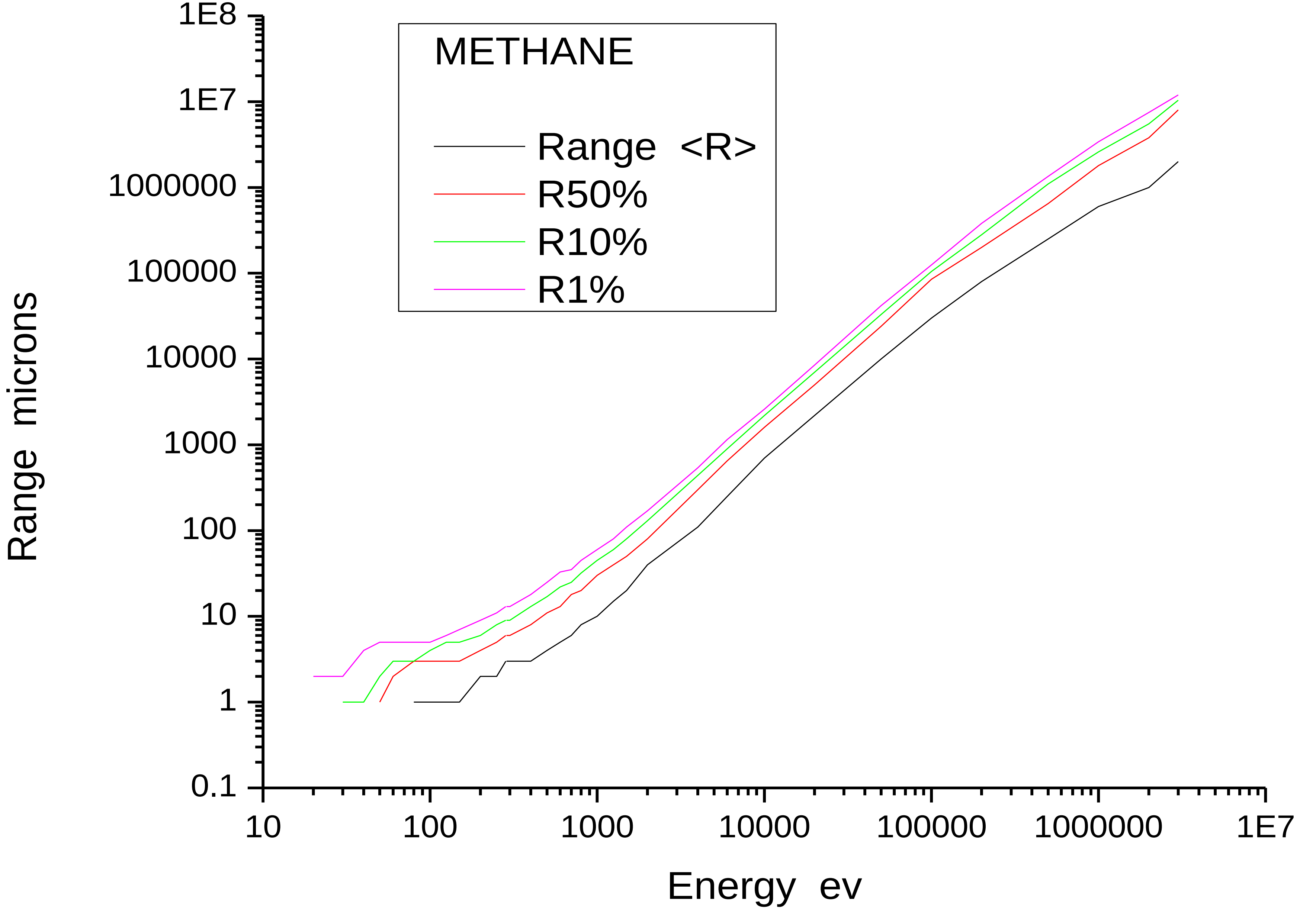


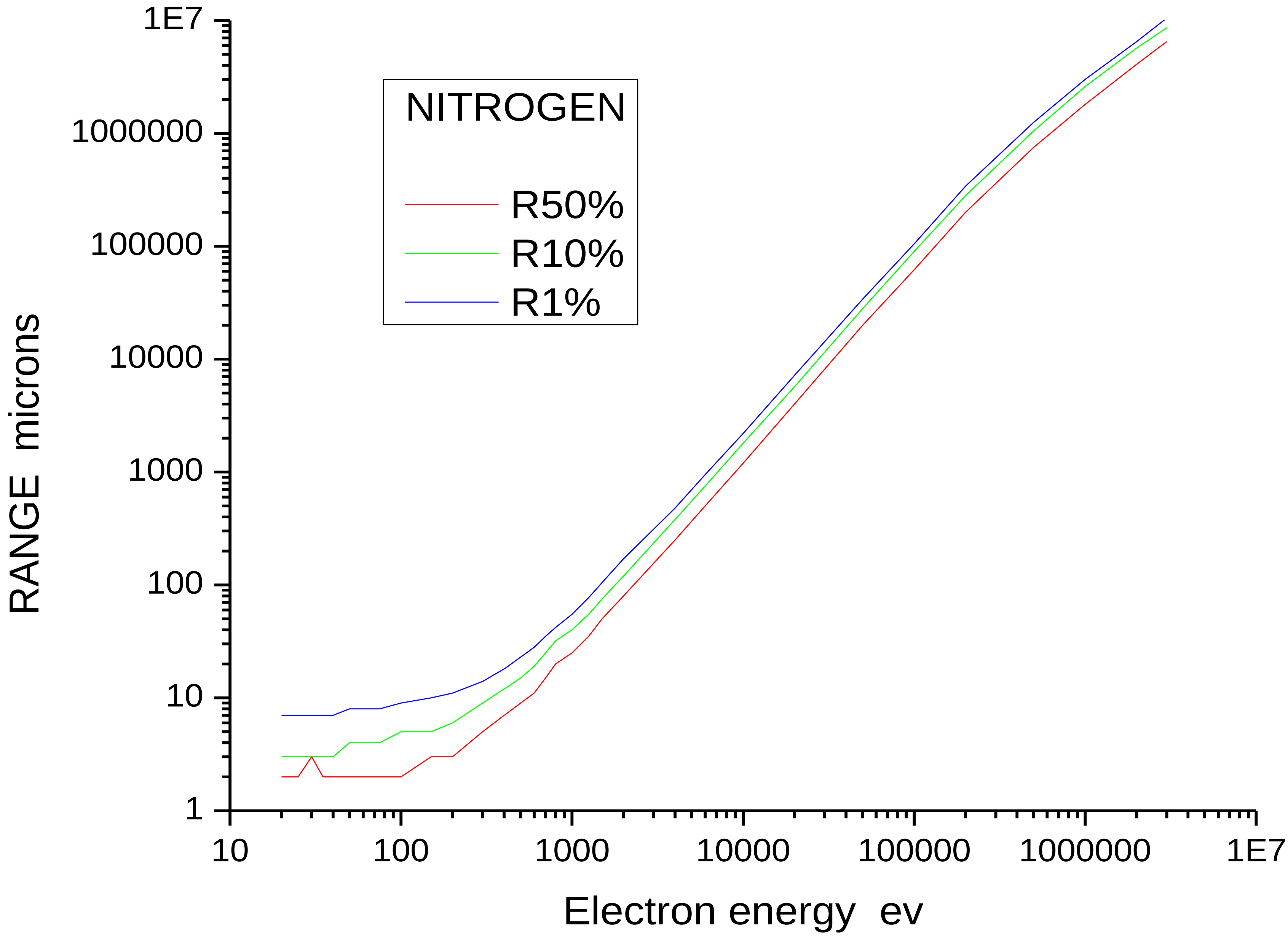
METHANE
x-ray
e-beam
weibel+grosswendt
combercher
W ev/ion pair
Energy ev
70
60
50
40
30
20
10
10
100
1000
10000
100000
1000000

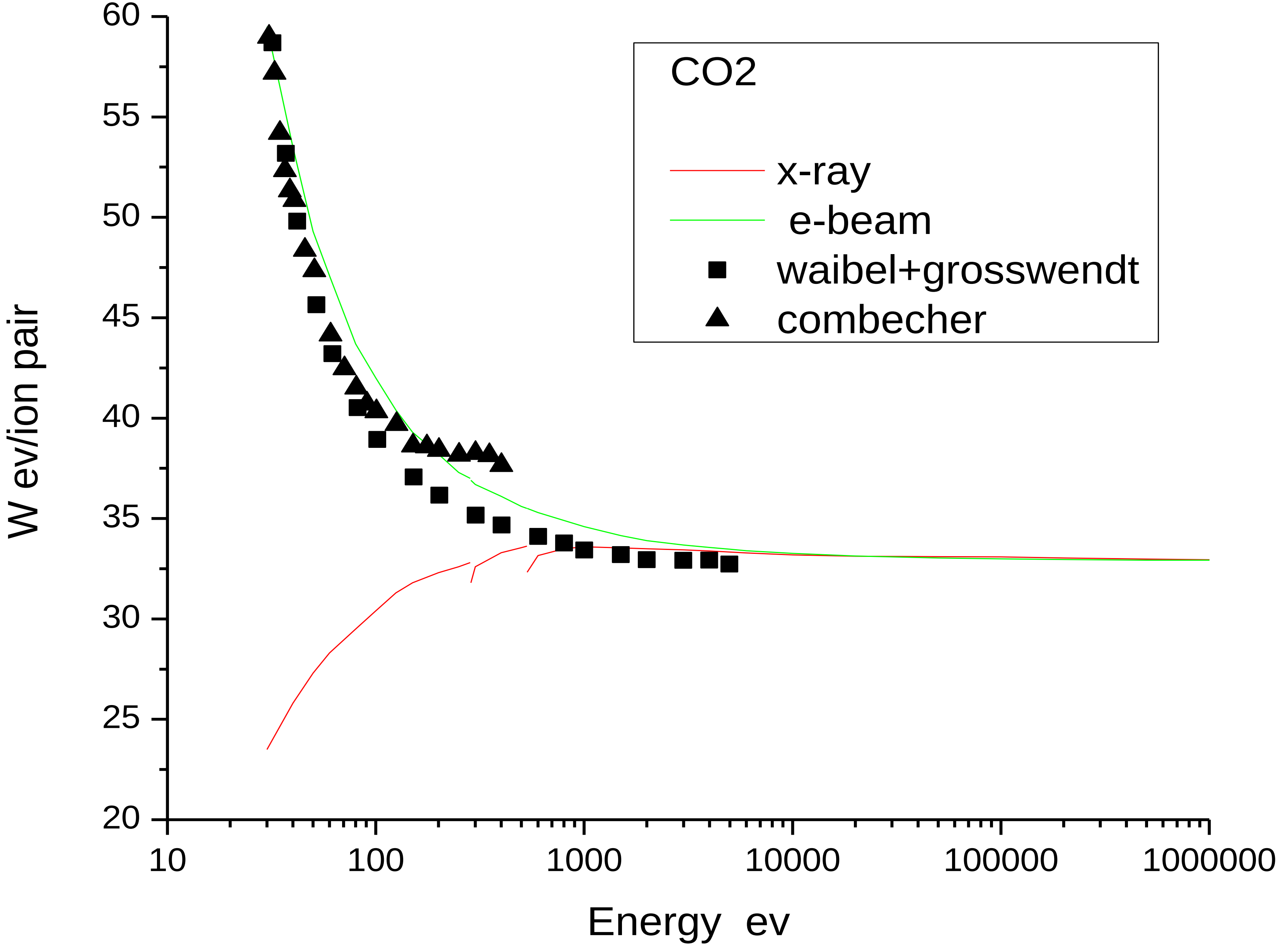


METHANE
x-ray
e-beam
Fano
0.7
0.6
0.5
0.4
0.3
0.2
0.1
10
100
1000
10000
100000
1000000
Energy ev

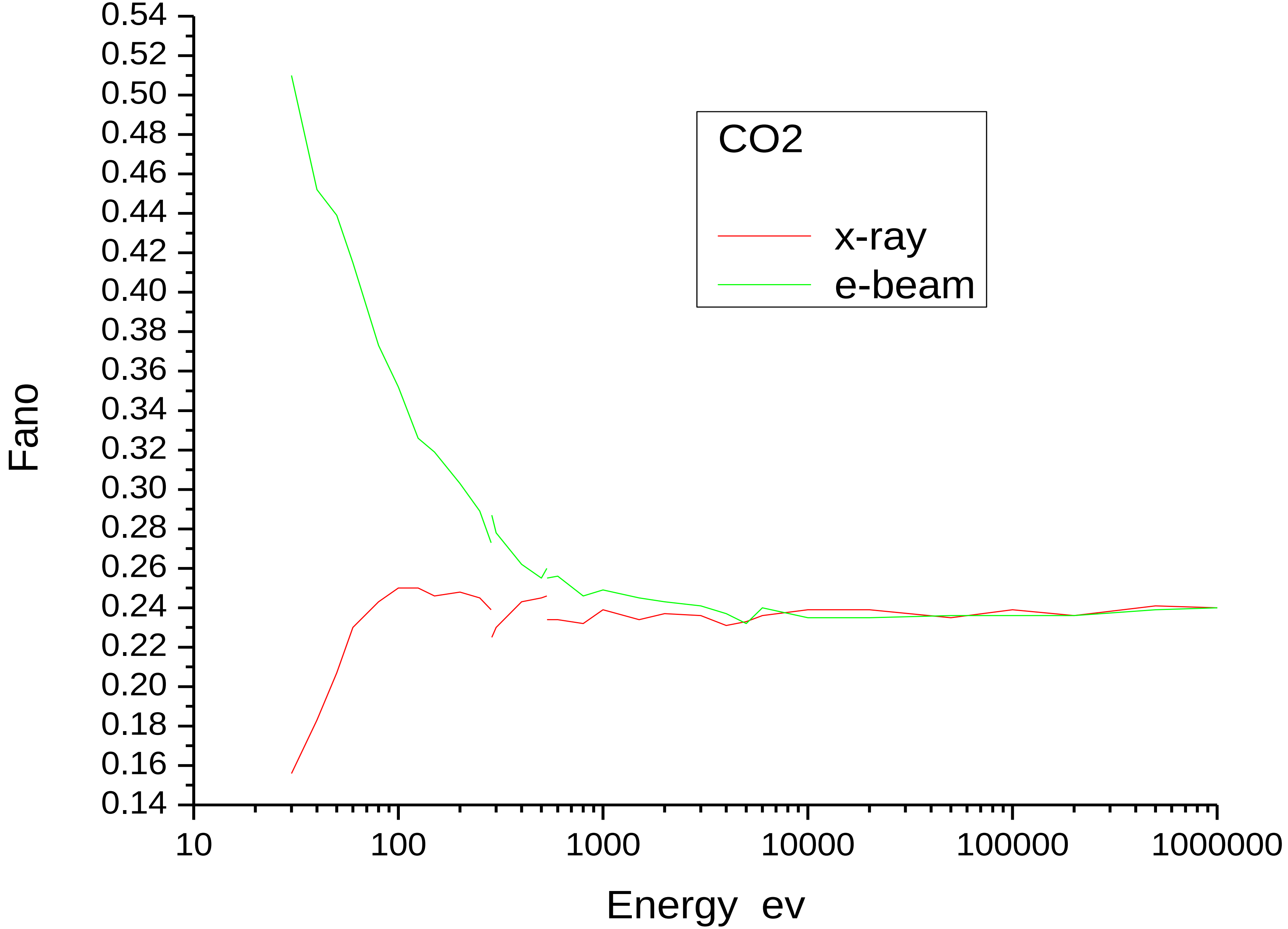

METHANE
abs length
P.E.abs length mm.
Energy ev
1000000
100000
10000
1000
100
10
1
0.1
0.01
10
100
1000
10000
100000
1000000


METHANE
Range <R>
R50%
R10%
R1%
Range microns
Energy ev
1E8
1E7
1000000
100000
10000
1000
100
10
1
0.1
10
100
1000
10000
100000
1000000
1E7

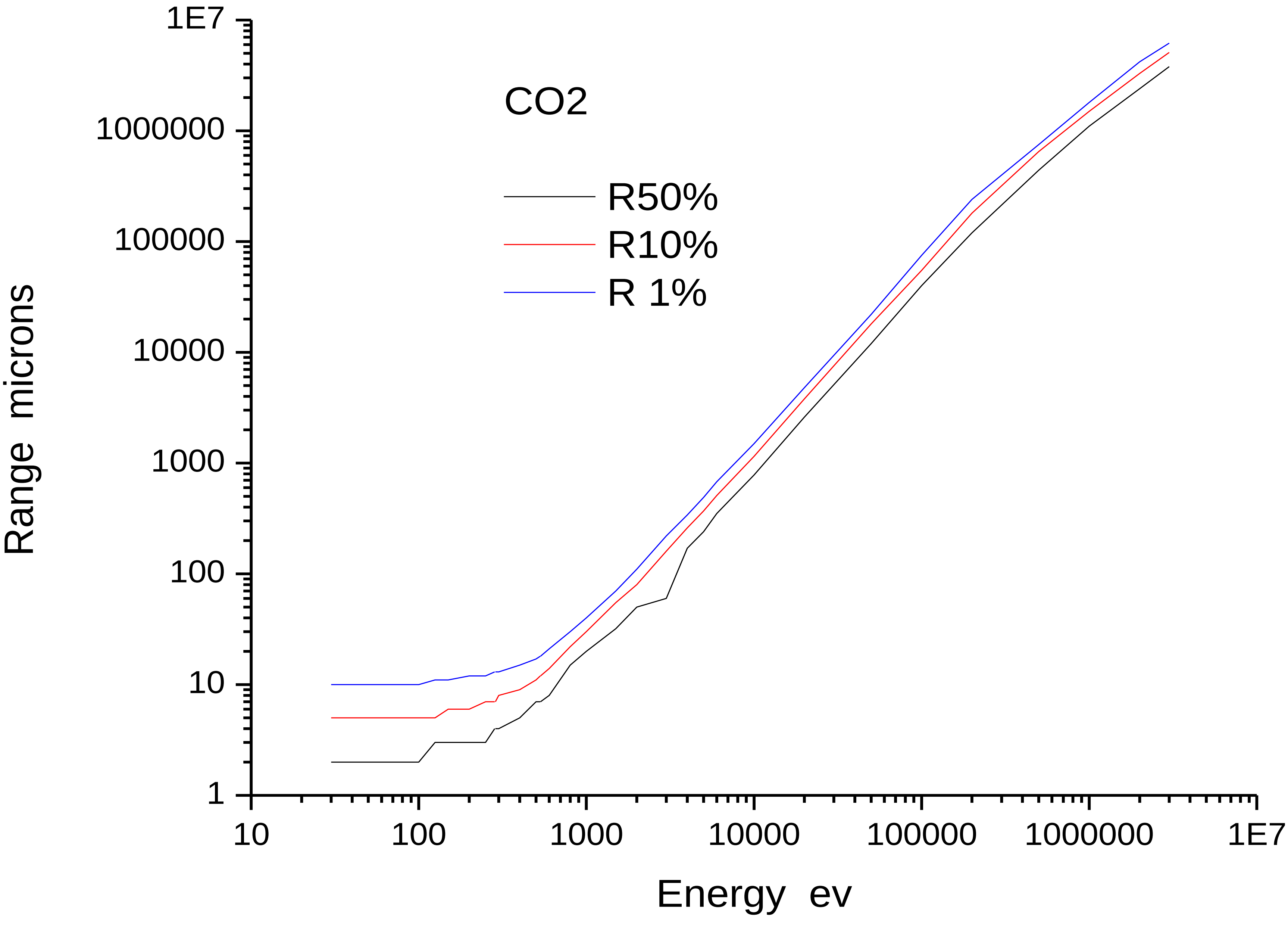

NITROGEN
R50%
R10%
R1%
1E7
1000000
100000
10000
1000
100
10
1
10
100
1000
10000
100000
1000000
1E7
RANGE microns
Electron energy ev



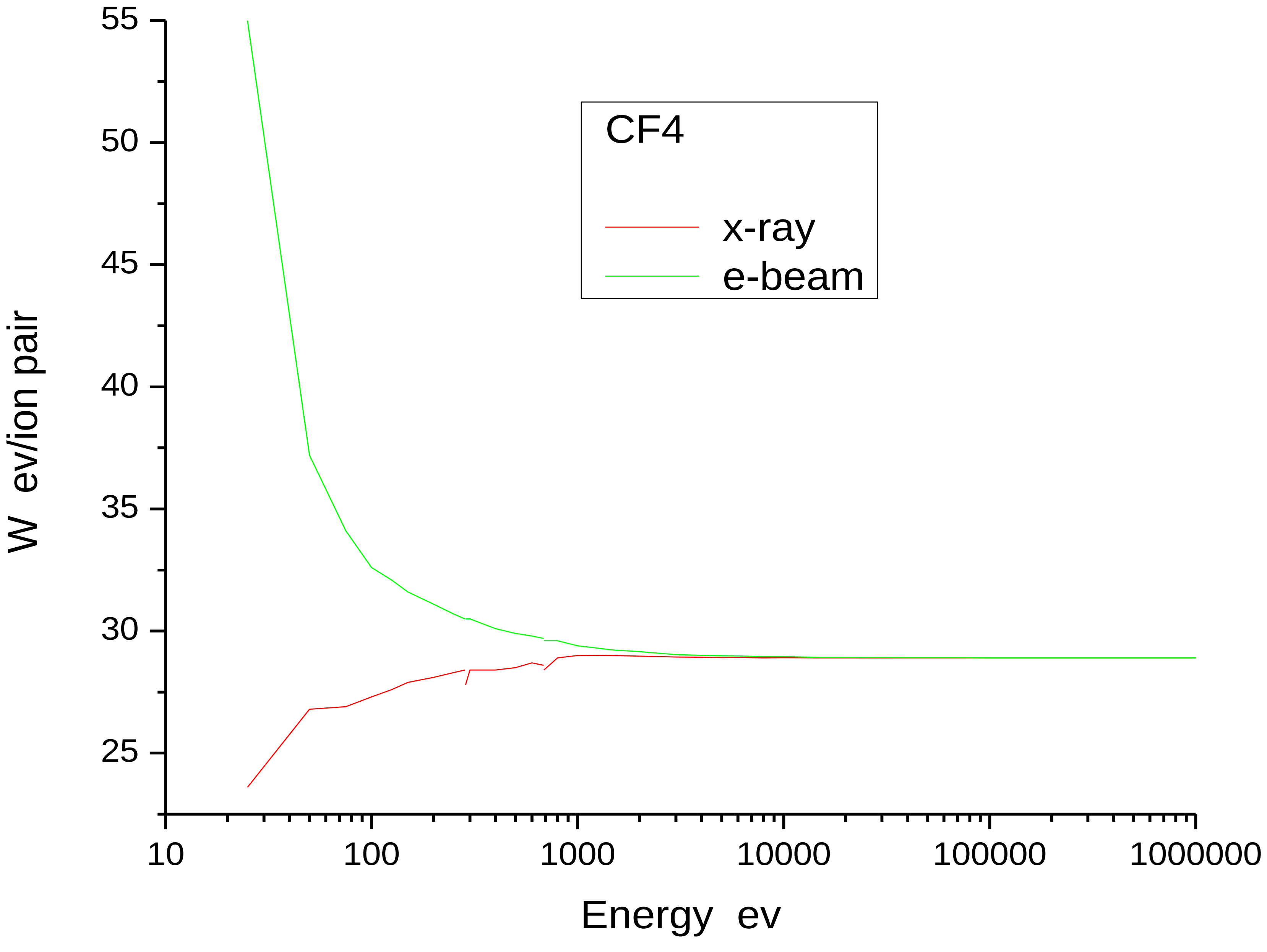
CO2
x-ray
e-beam
waibel+grosswendt
combecher
W ev/ion pair
Energy ev
60
55
50
45
40
35
30
25
20
10
100
1000
10000
100000
1000000



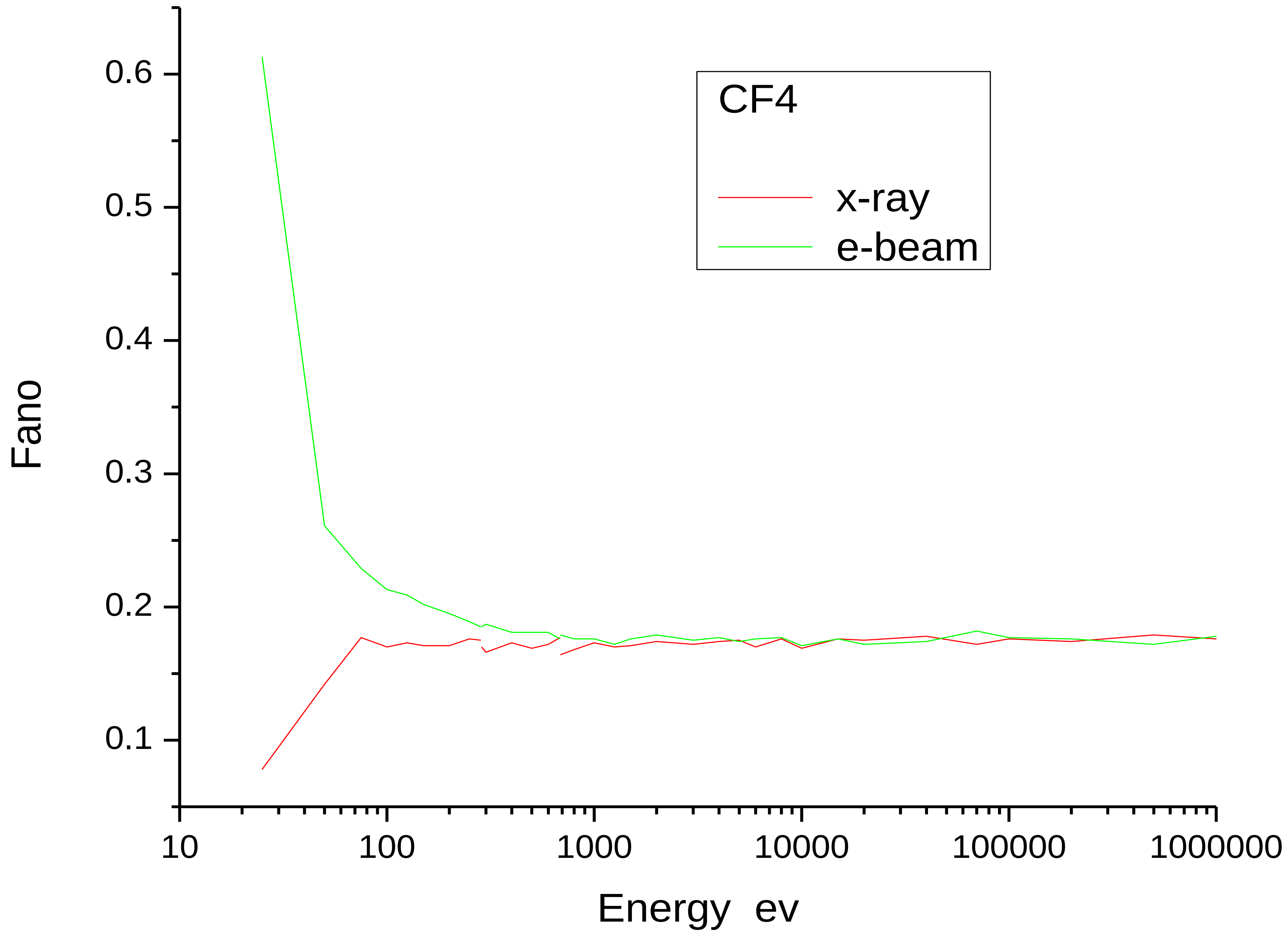
CO2
x-ray
e-beam
Fano
Energy ev
0.54
0.52
0.50
0.48
0.46
0.44
0.42
0.40
0.38
0.36
0.34
0.32
0.30
0.28
0.26
0.24
0.22
0.20
0.18
0.16
0.14
10
100
1000
10000
100000
1000000



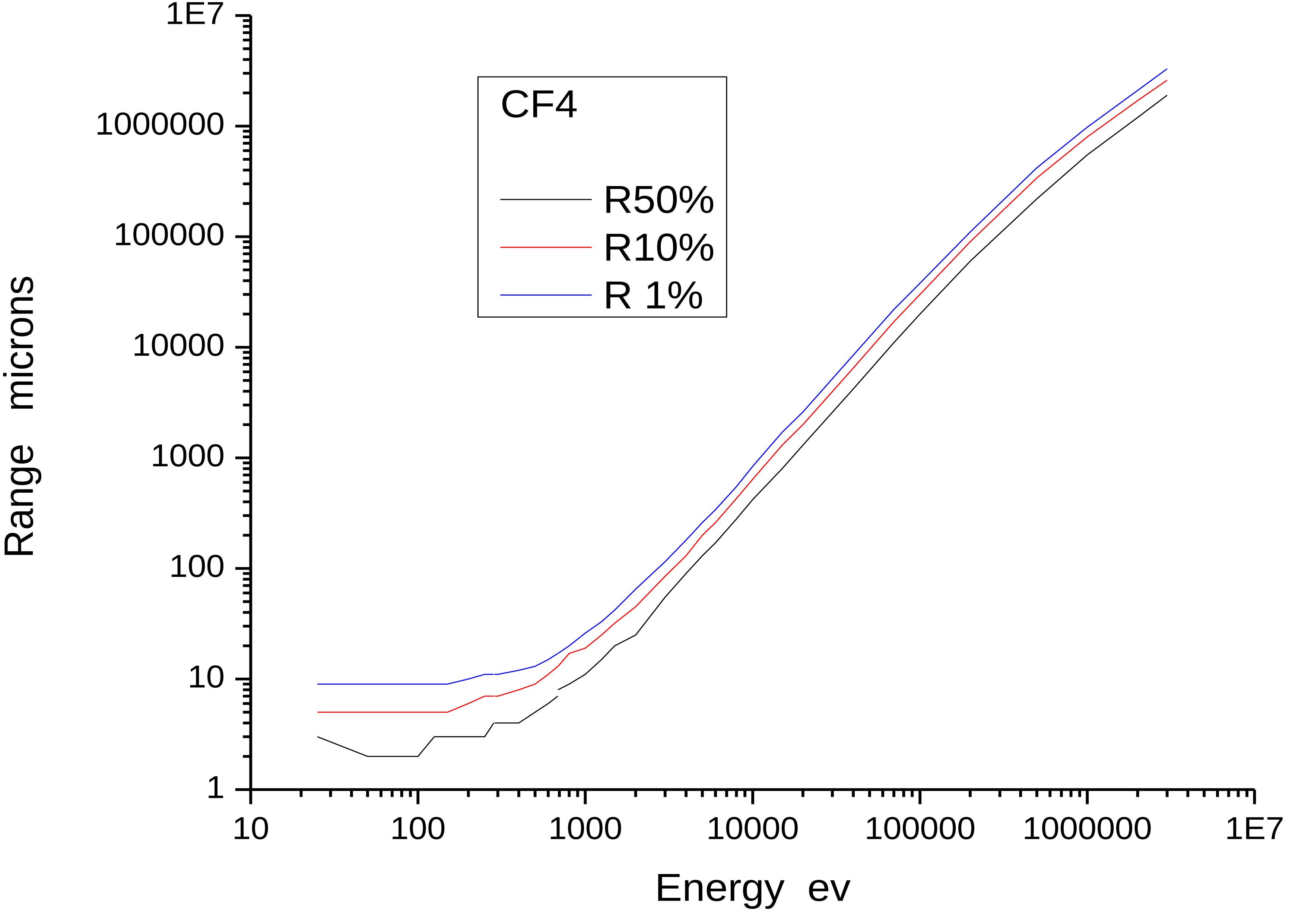
CO2
R50%
R10%
R 1%
Range microns
Energy ev
1E7
1000000
100000
10000
1000
100
10
1
10
100
1000
10000
100000
1000000
1E7

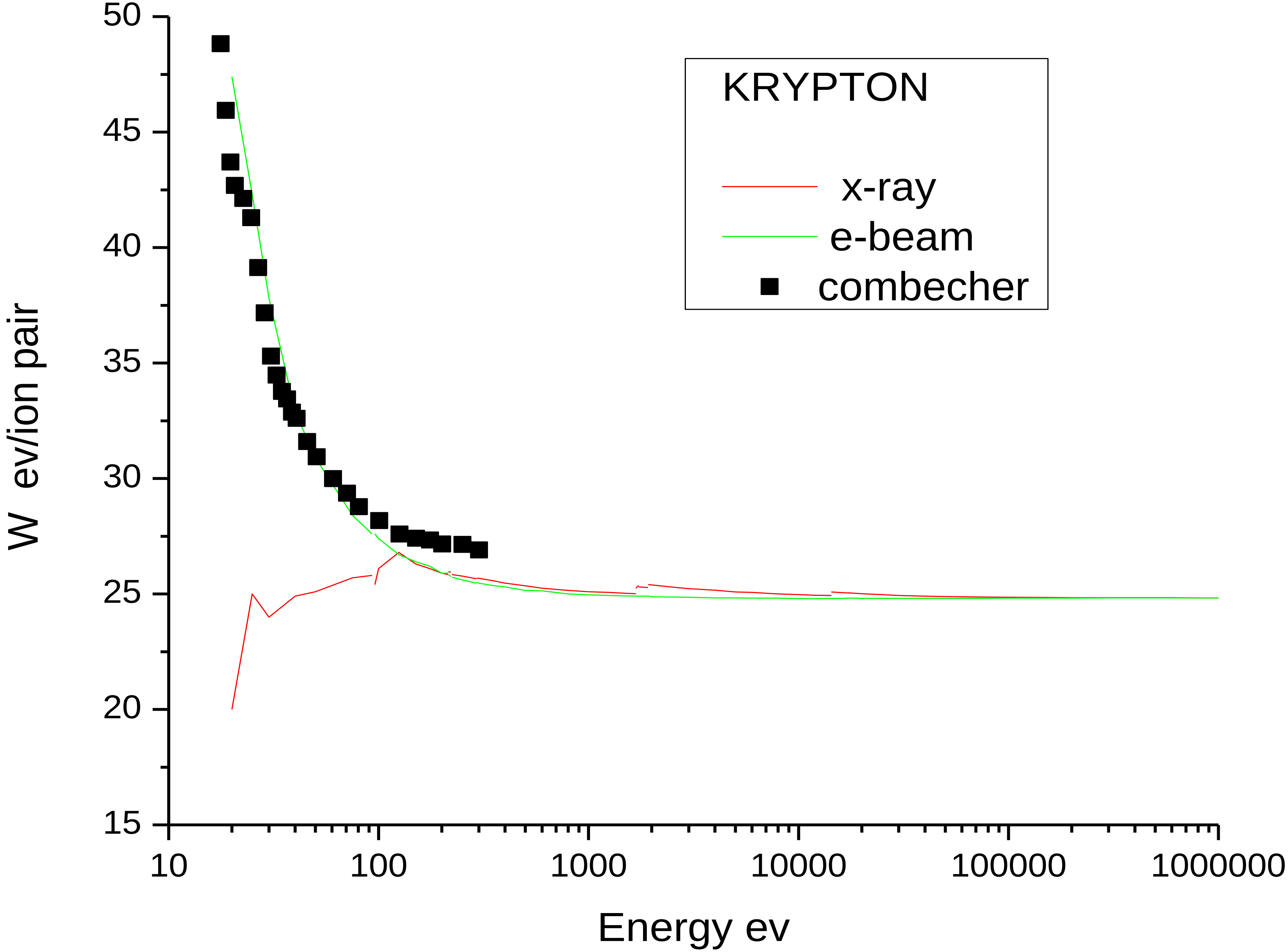


CF4
x-ray
e-beam
55
50
45
40
35
30
25
W ev/ion pair
10
100
1000
10000
100000
1000000
Energy ev

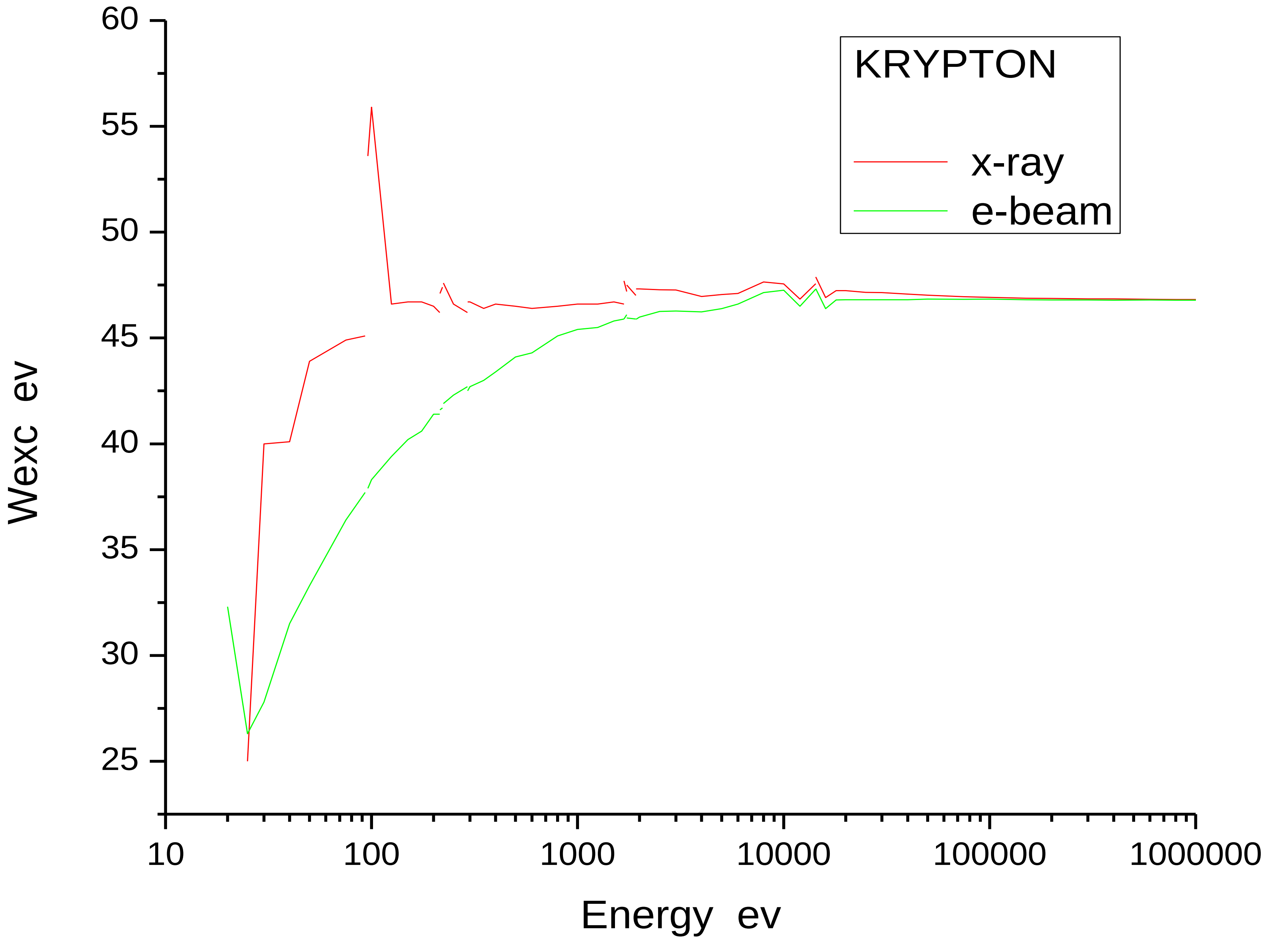


CF4
x-ray
e-beam
Fano
0.1
0.2
0.3
0.4
0.5
0.6
10
100
1000
10000
100000
1000000
Energy ev

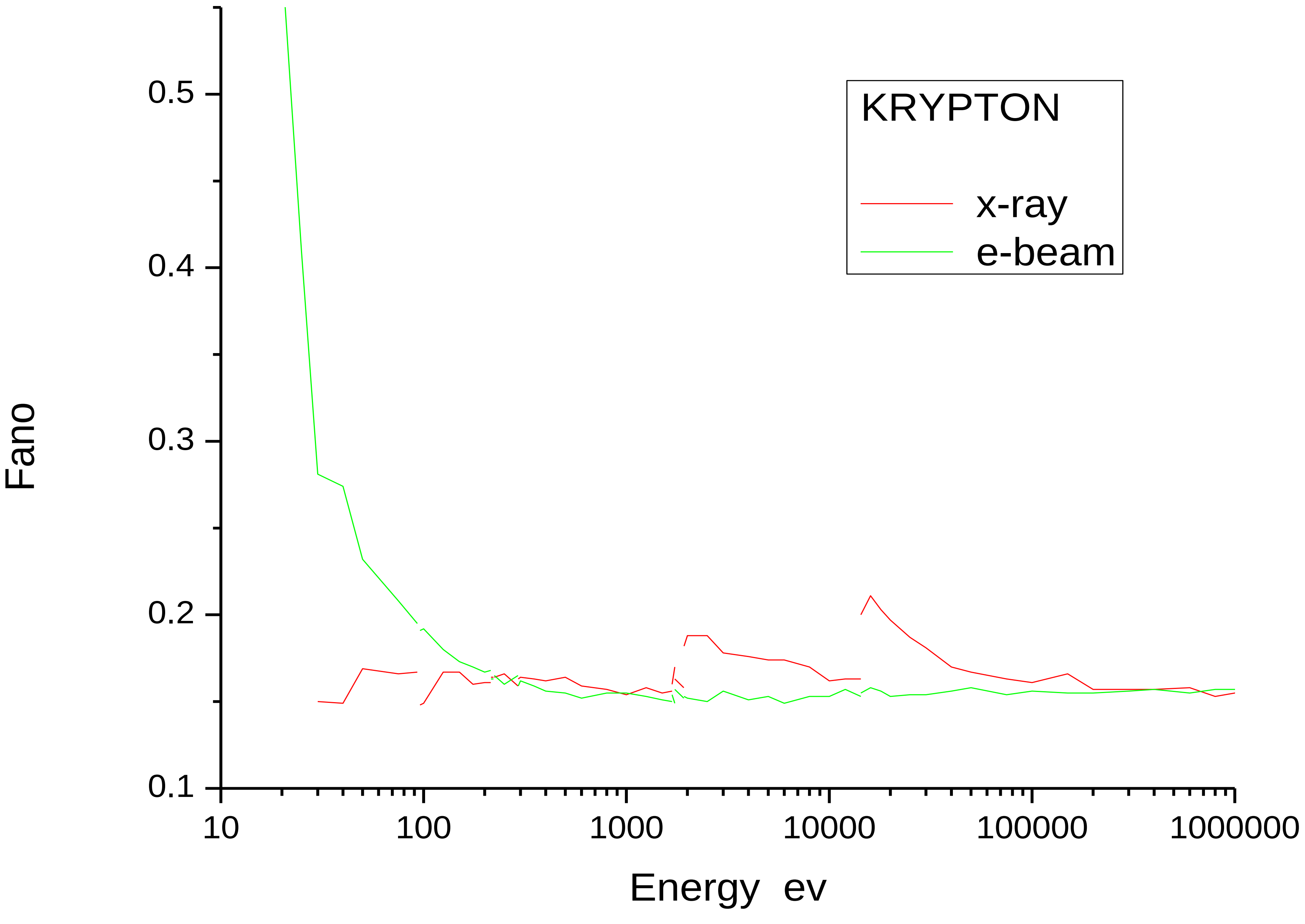

CF4
R50%
R10%
R 1%
1E7
1000000
100000
10000
1000
100
10
1
10
100
1000
10000
100000
1000000
1E7
Range microns
Energy ev



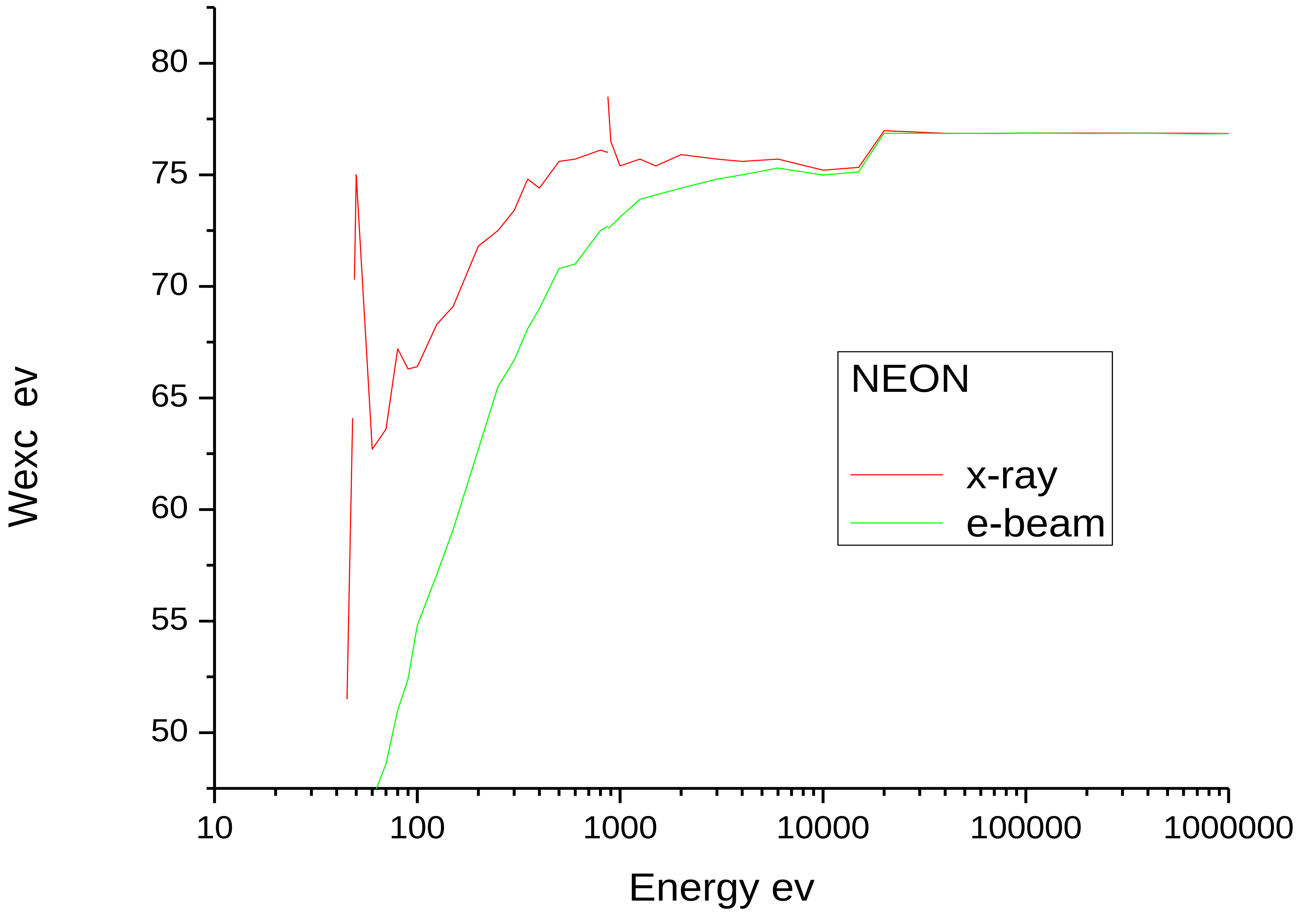
KRYPTON
x-ray
e-beam
combecher
W ev/ion pair
Energy ev
50
45
40
35
30
25
20
15
10
100
1000
10000
100000
1000000



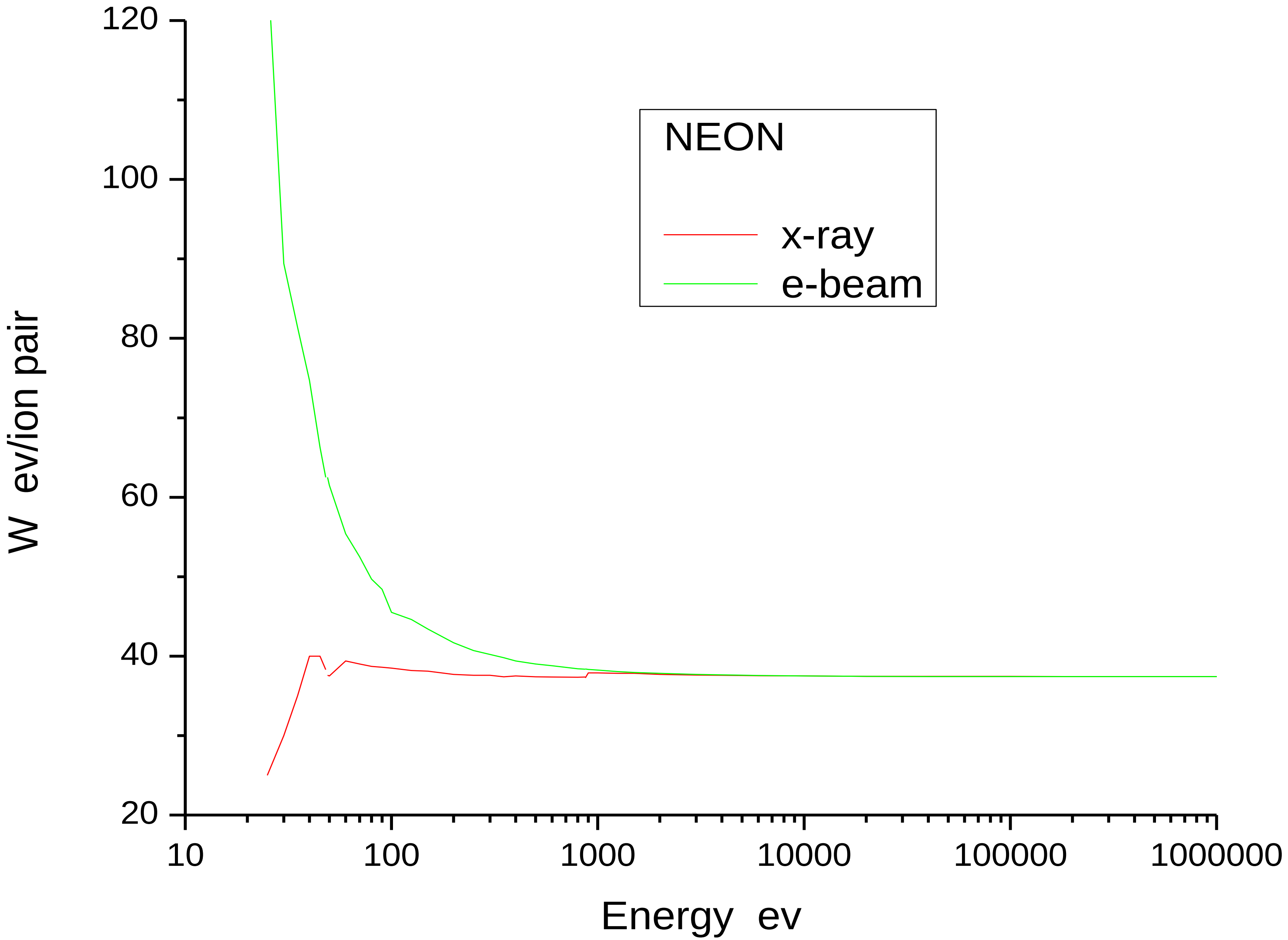
KRYPTON
x-ray
e-beam
Wexc ev
Energy ev
60
55
50
45
40
35
30
25
10
100
1000
10000
100000
1000000



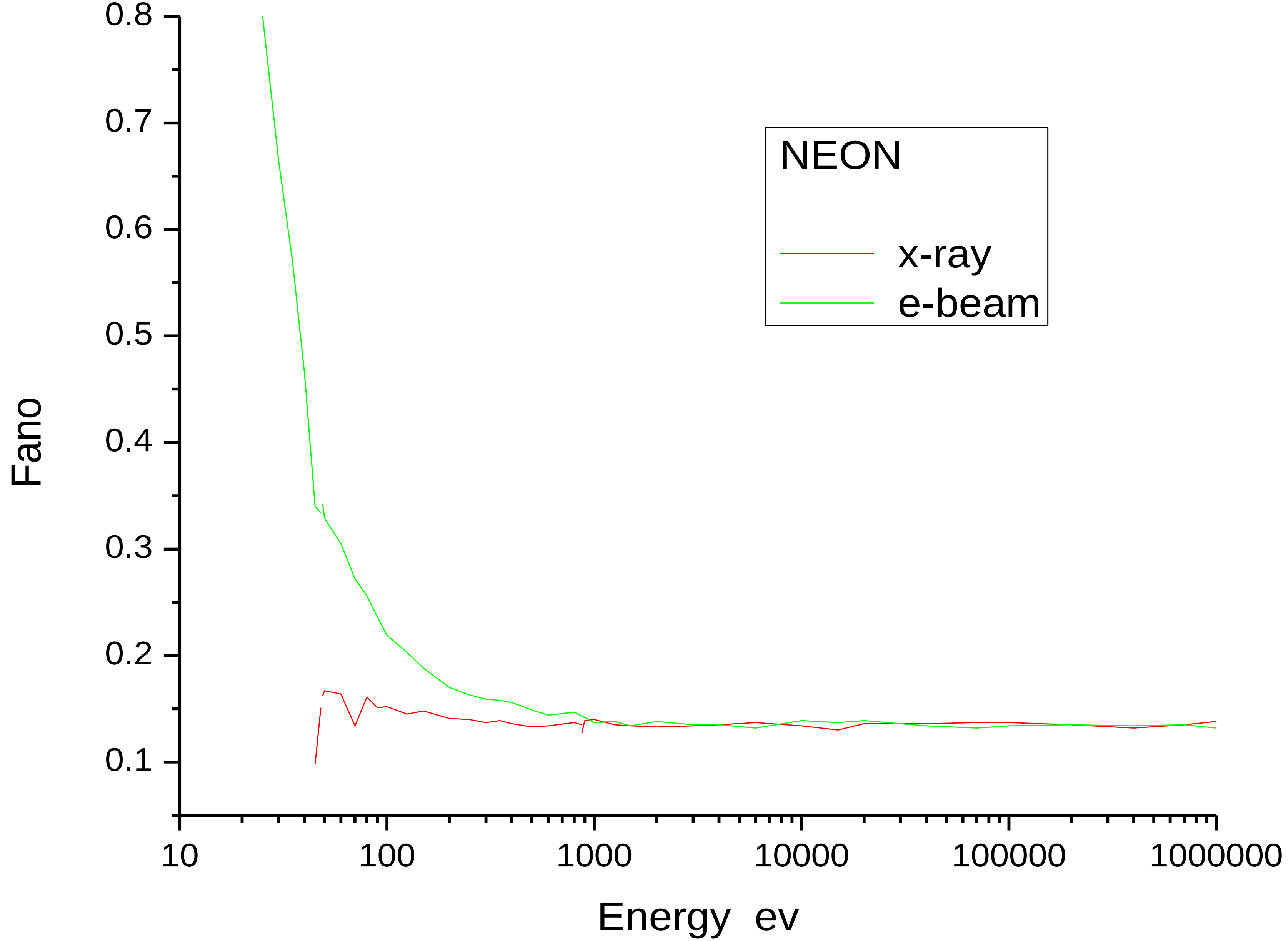
KRYPTON
x-ray
e-beam
Fano
0.1
0.2
0.3
0.4
0.5
10
100
1000
10000
100000
1000000
Energy ev



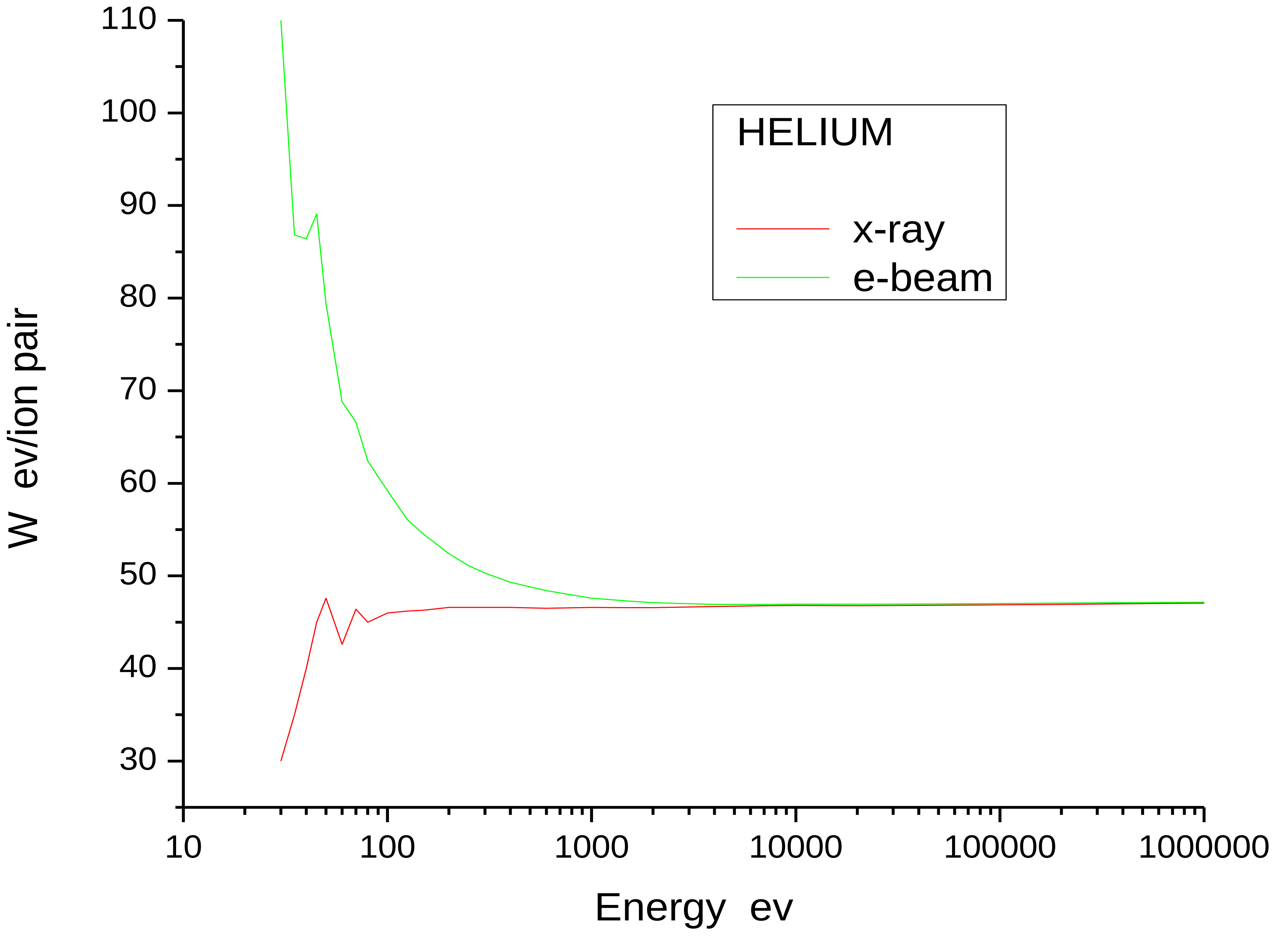
Wexc ev
80
75
70
65
60
55
50
10
100
1000
10000
100000
1000000
Energy ev
NEON
x-ray
e-beam

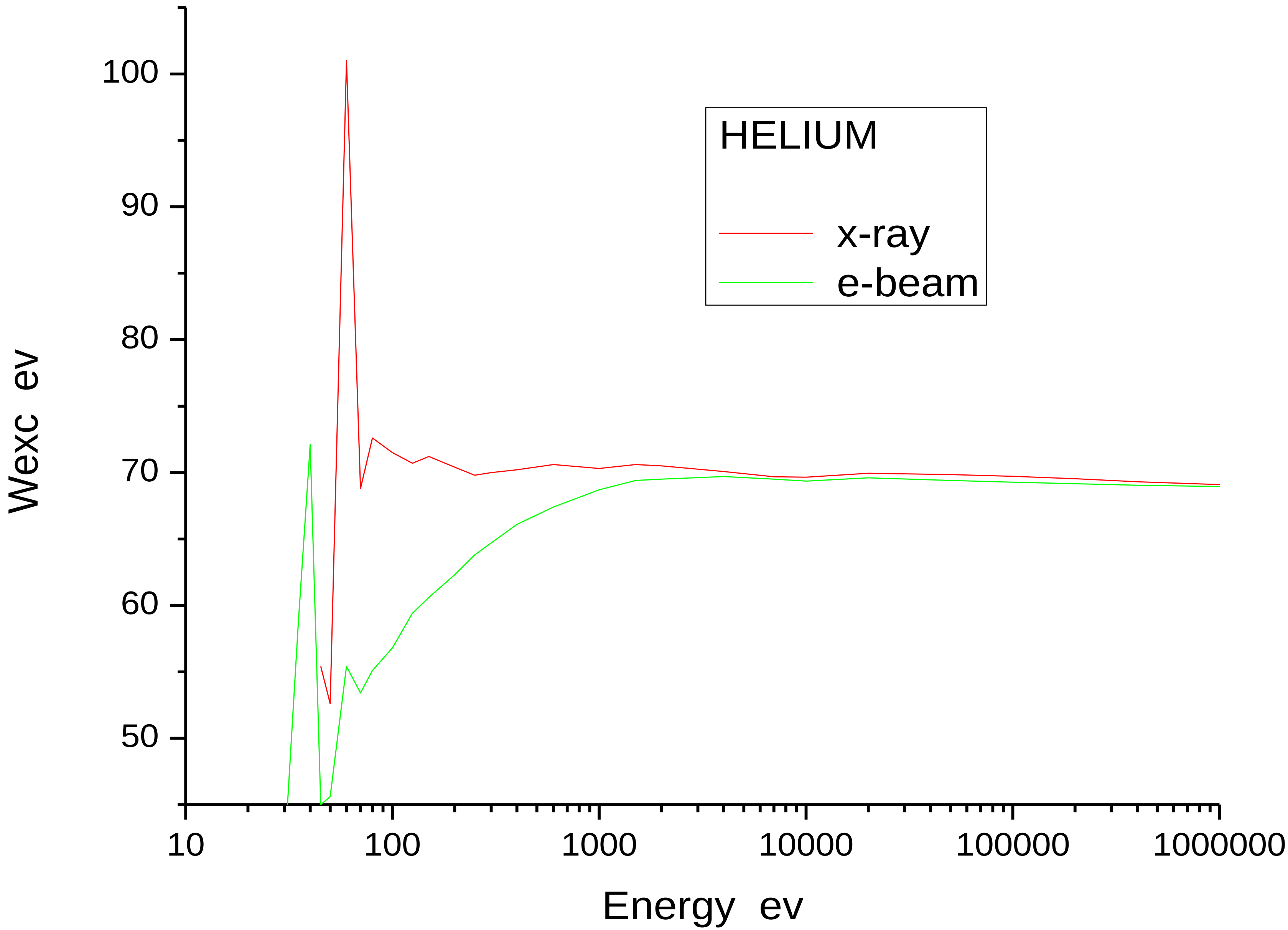


NEON
x-ray
e-beam
120
100
80
60
40
20
W ev/ion pair
10
100
1000
10000
100000
1000000
Energy ev

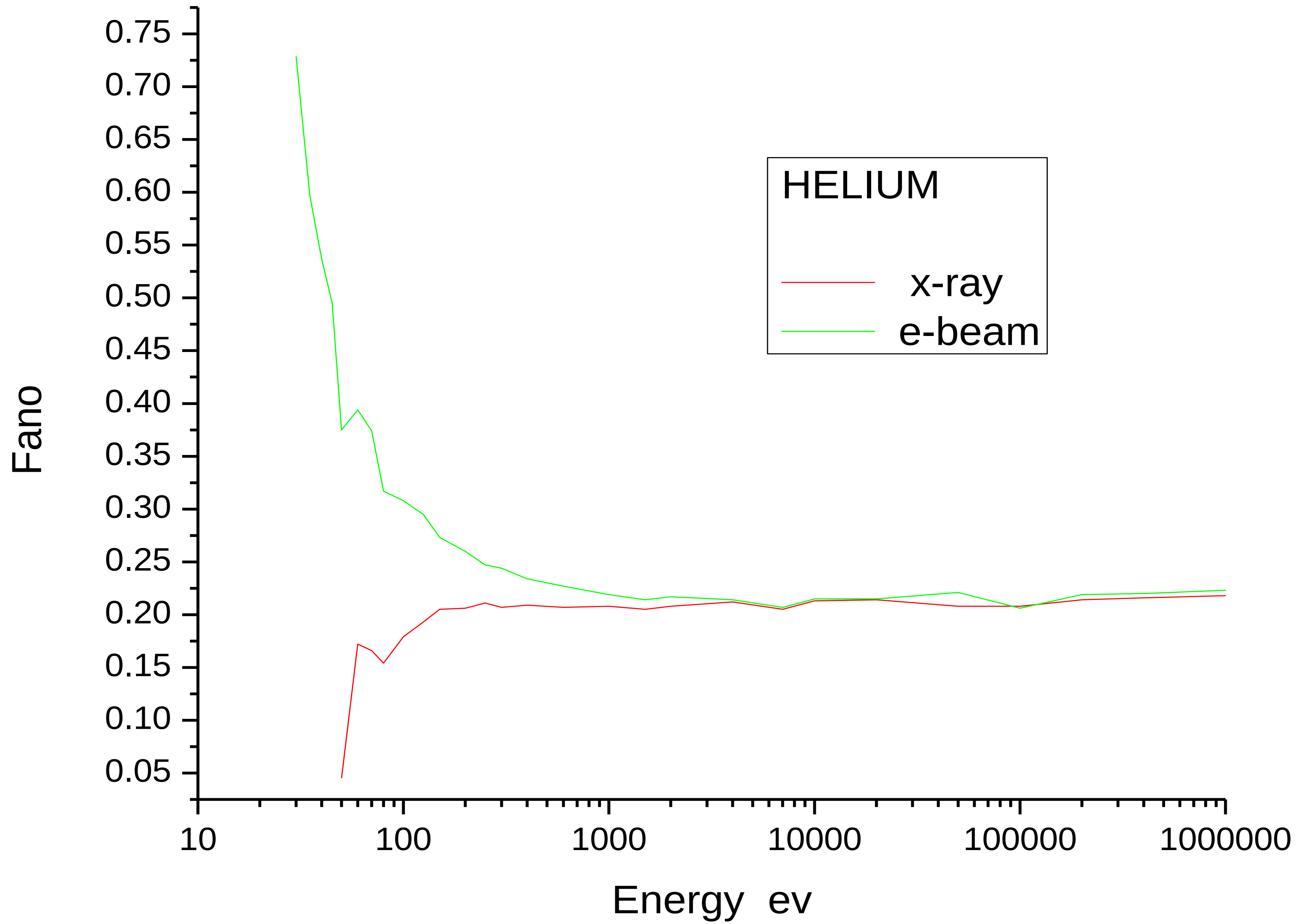


NEON
x-ray
e-beam
Fano
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
10
100
1000
10000
100000
1000000
Energy ev

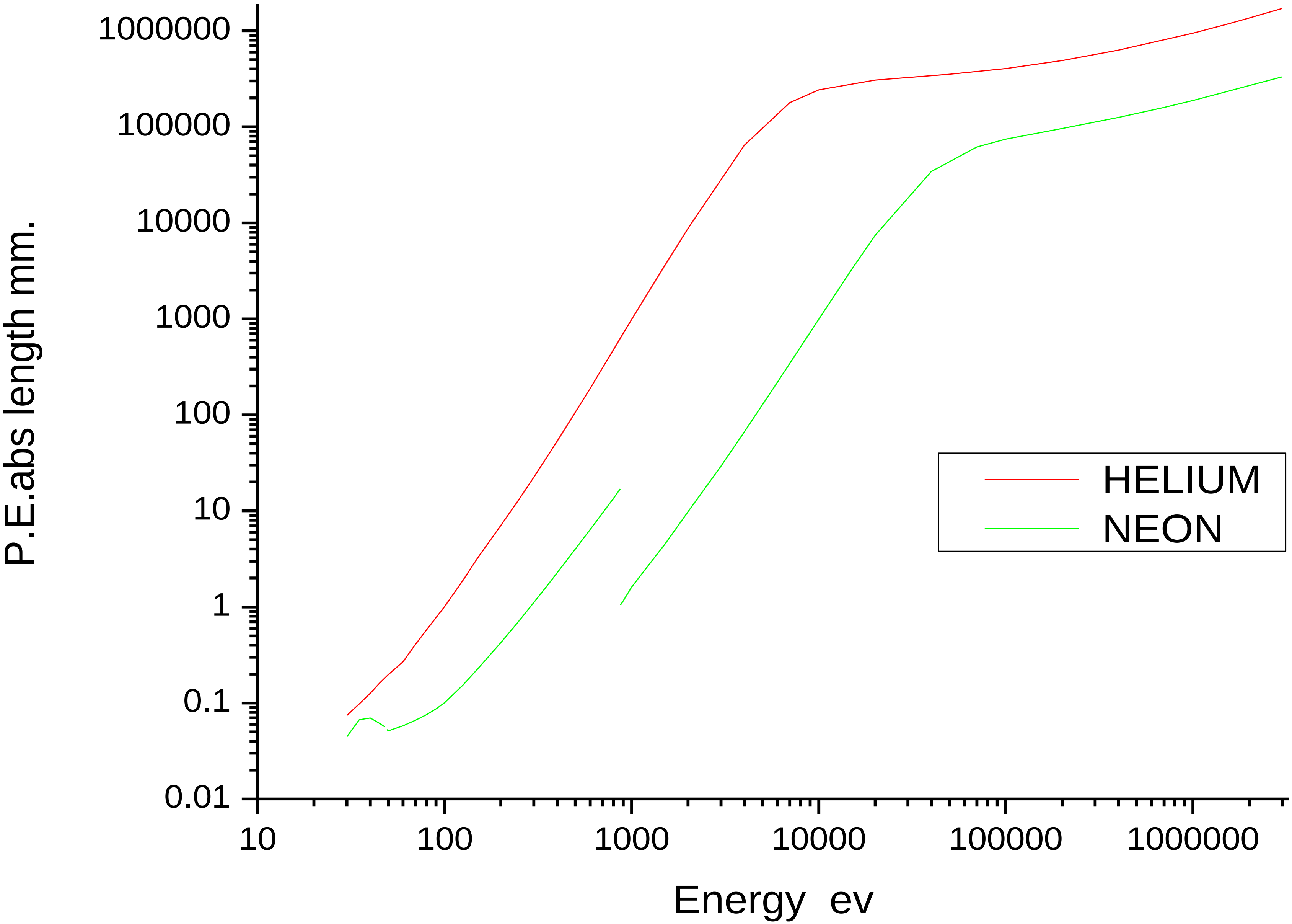

HELIUM
x-ray
e-beam
W ev/ion pair
Energy ev
110
100
90
80
70
60
50
40
30
10
100
1000
10000
100000
1000000



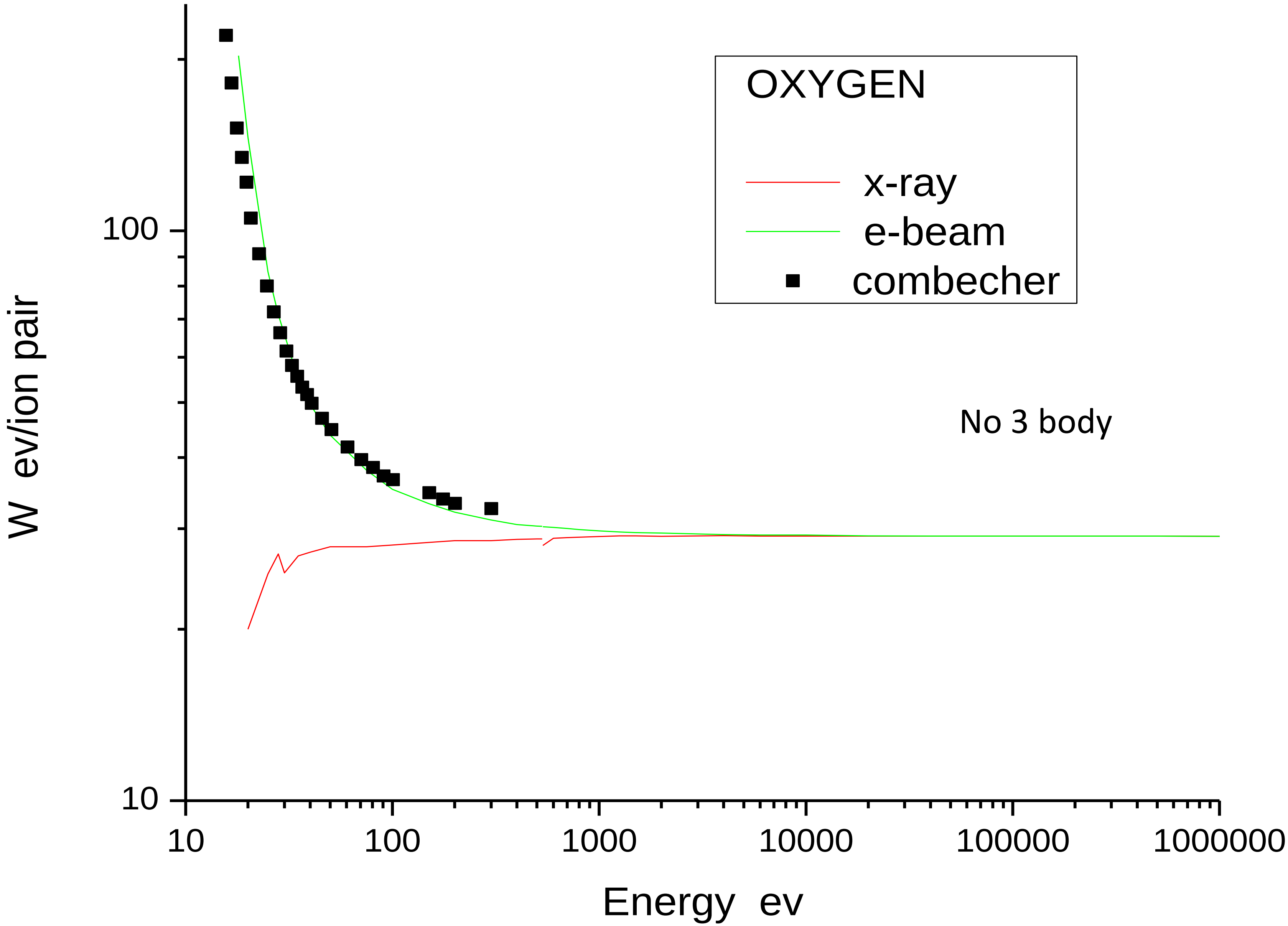
HELIUM
x-ray
e-beam
Wexc ev
Energy ev
100
90
80
70
60
50
10
100
1000
10000
100000
1000000



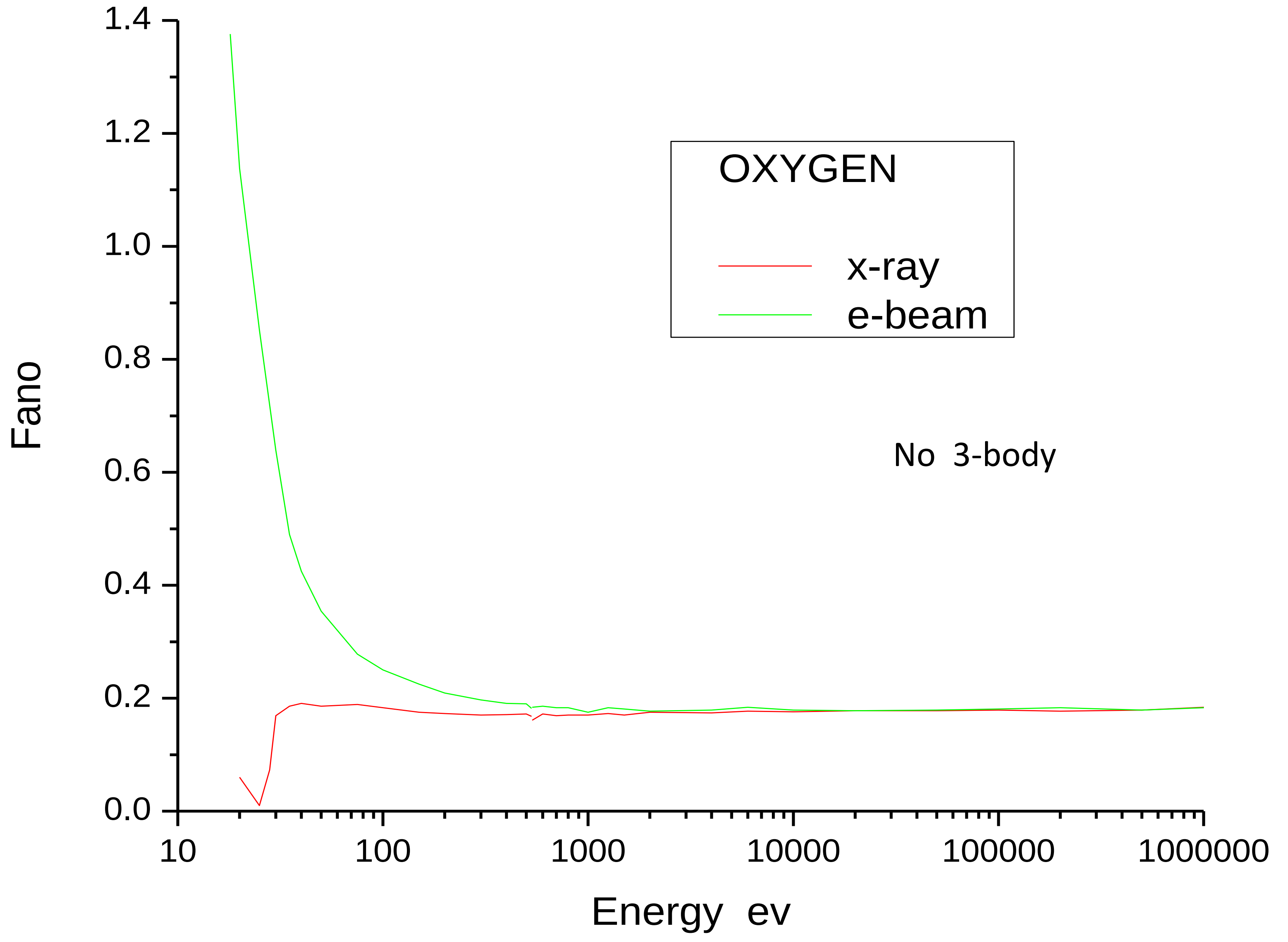
HELIUM
x-ray
e-beam
Fano
Energy ev
0.75
0.70
0.65
0.60
0.55
0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
10
100
1000
10000
100000
1000000



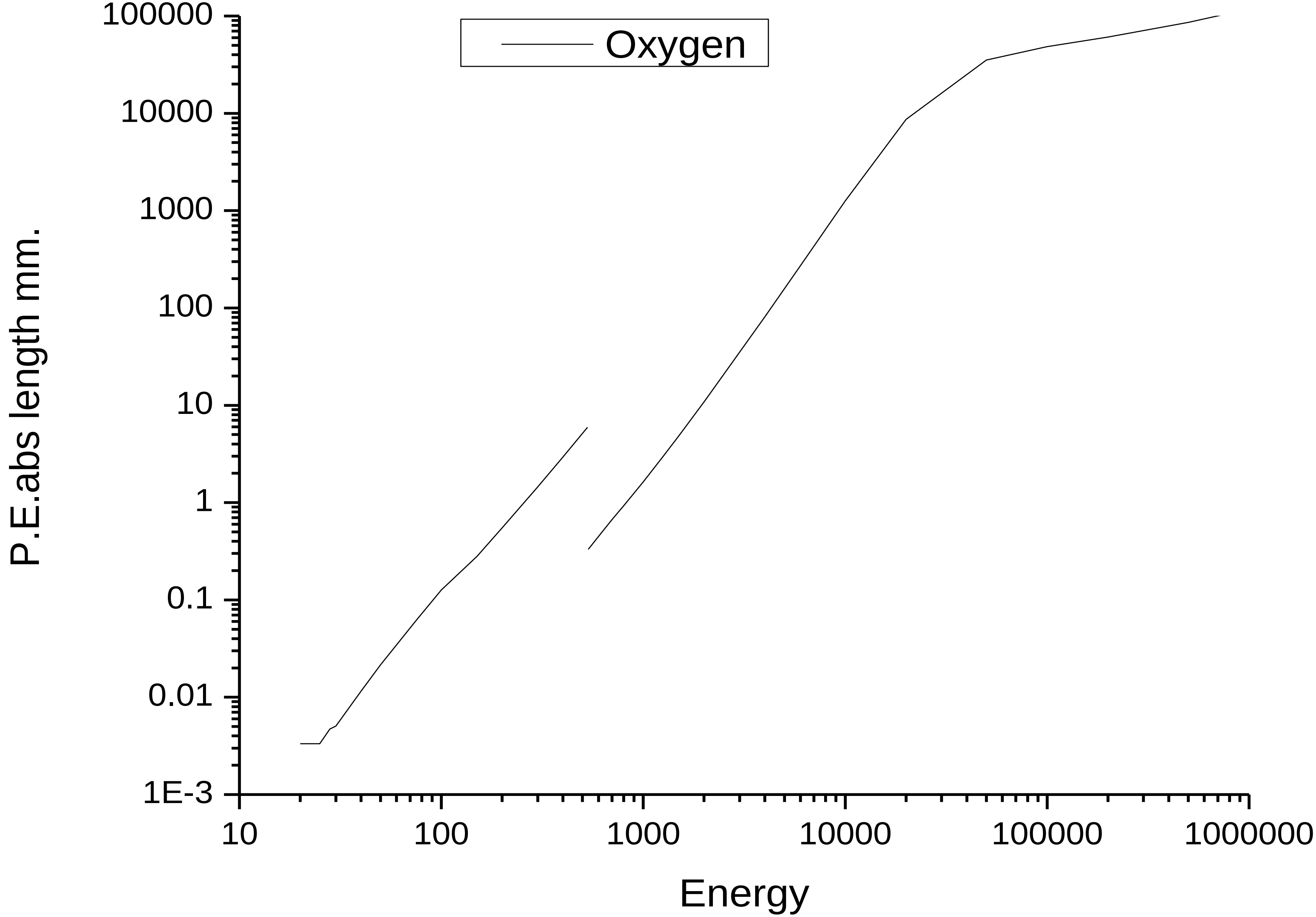
P.E.abs length mm.
1000000
100000
10000
1000
100
10
1
0.1
0.01
10
100
1000
10000
100000
1000000
Energy ev
HELIUM
NEON

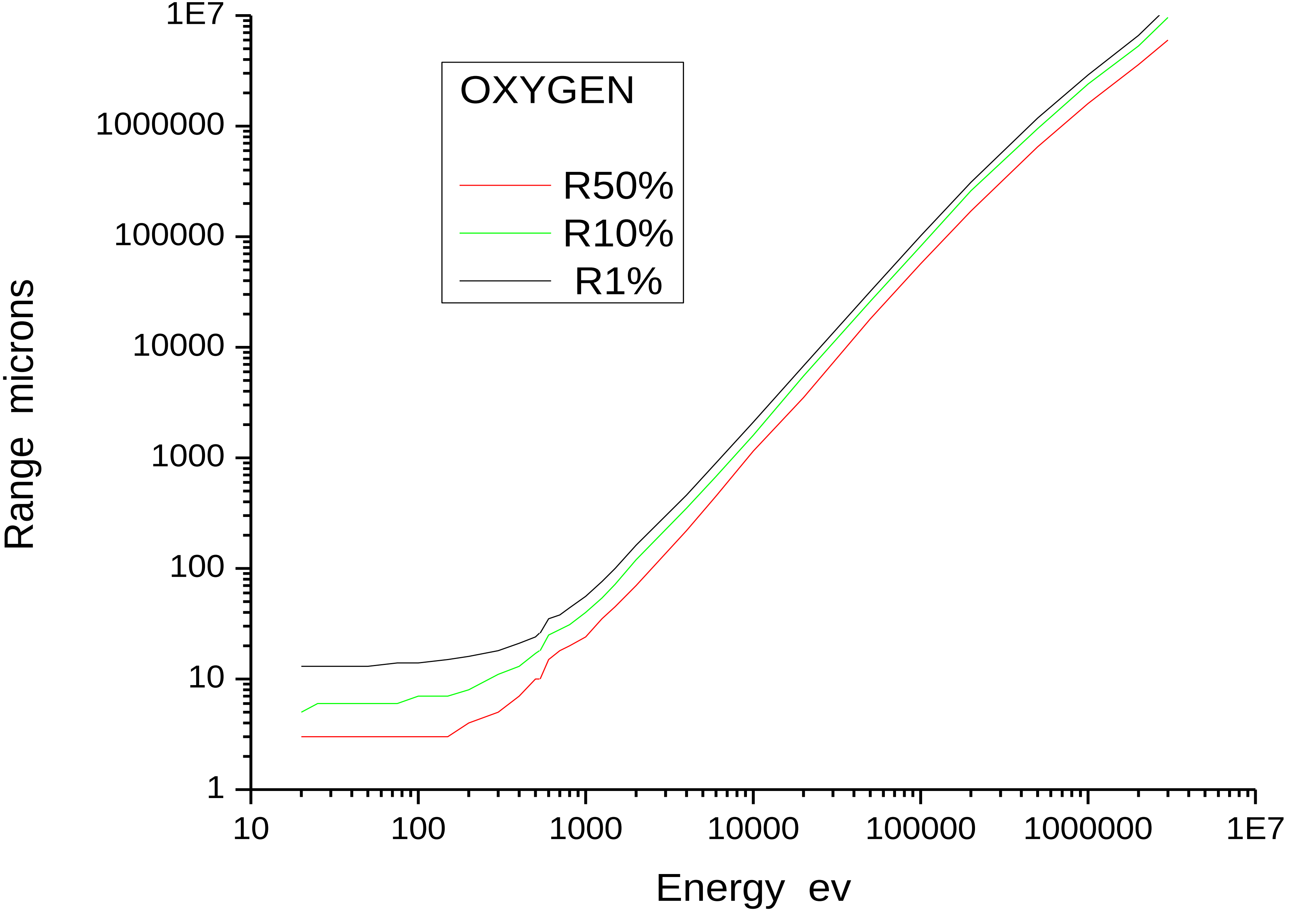


OXYGEN
x-ray
e-beam
combecher
No 3 body
W ev/ion pair
100
10
10
100
1000
10000
100000
1000000
Energy ev

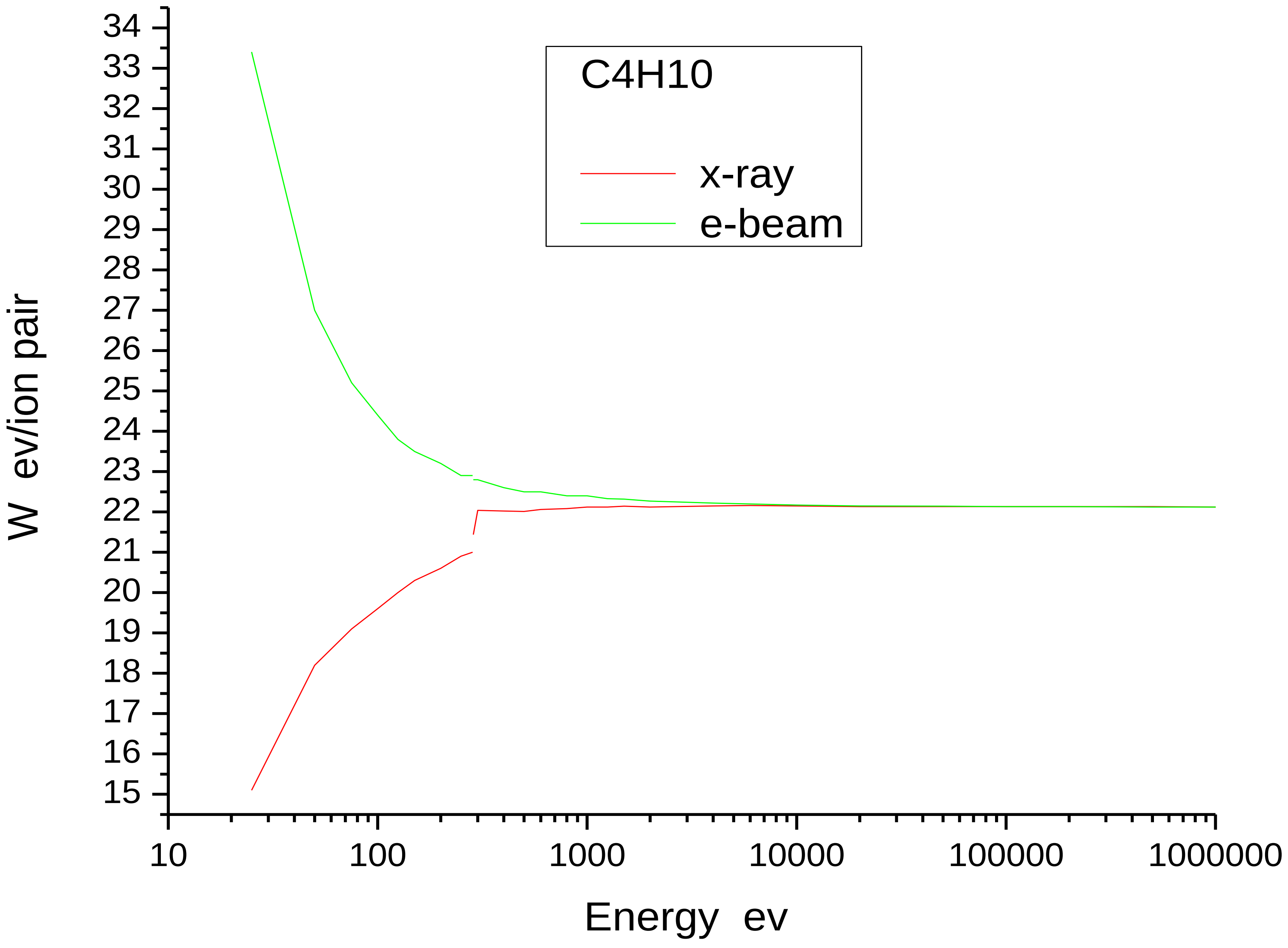


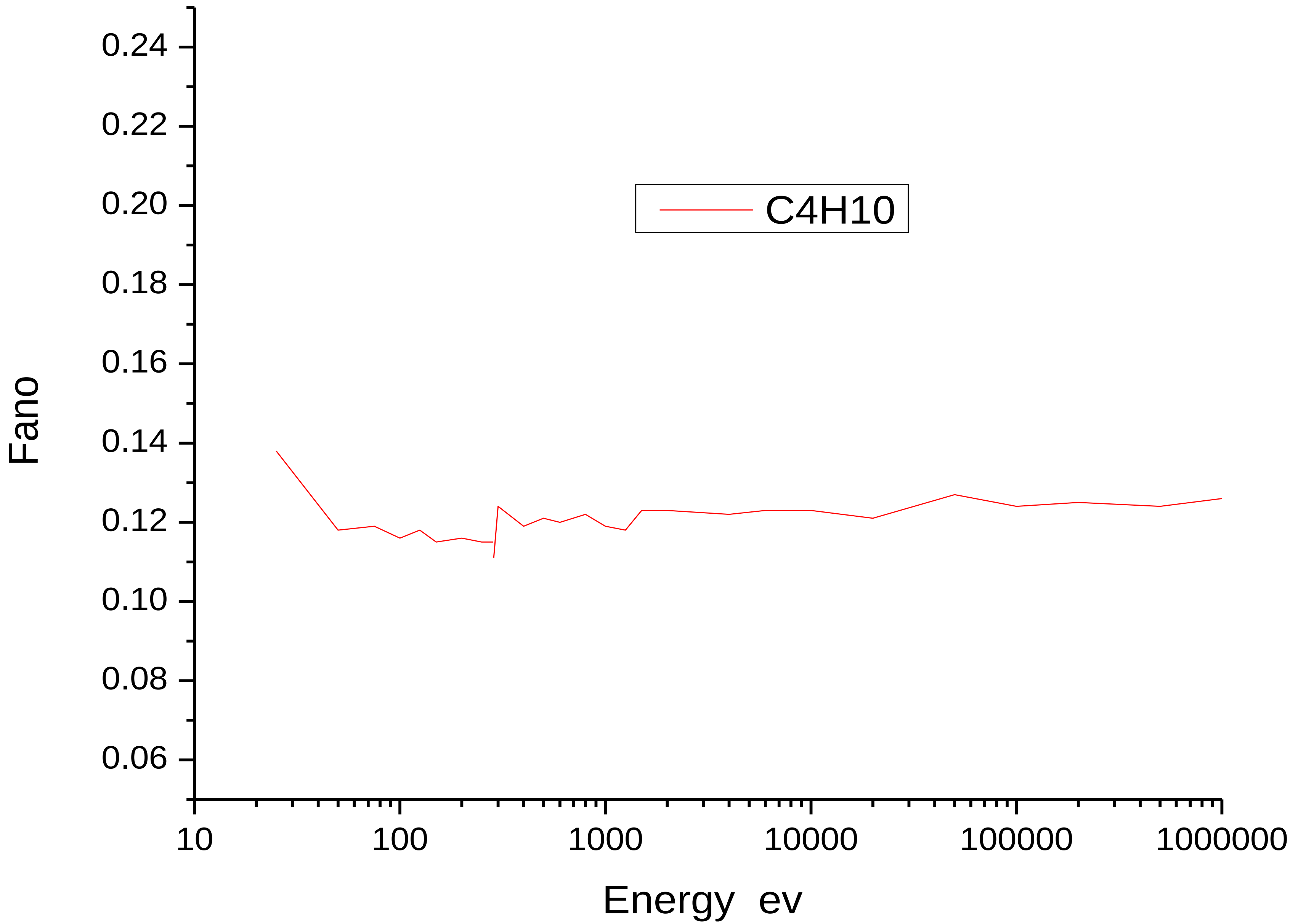
OXYGEN
x-ray
e-beam
No 3-body
Fano
Energy ev
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
10
100
1000
10000
100000
1000000


Oxygen
P.E.abs length mm.
100000
10000
1000
100
10
1
0.1
0.01
1E-3
10
100
1000
10000
100000
1000000
Energy

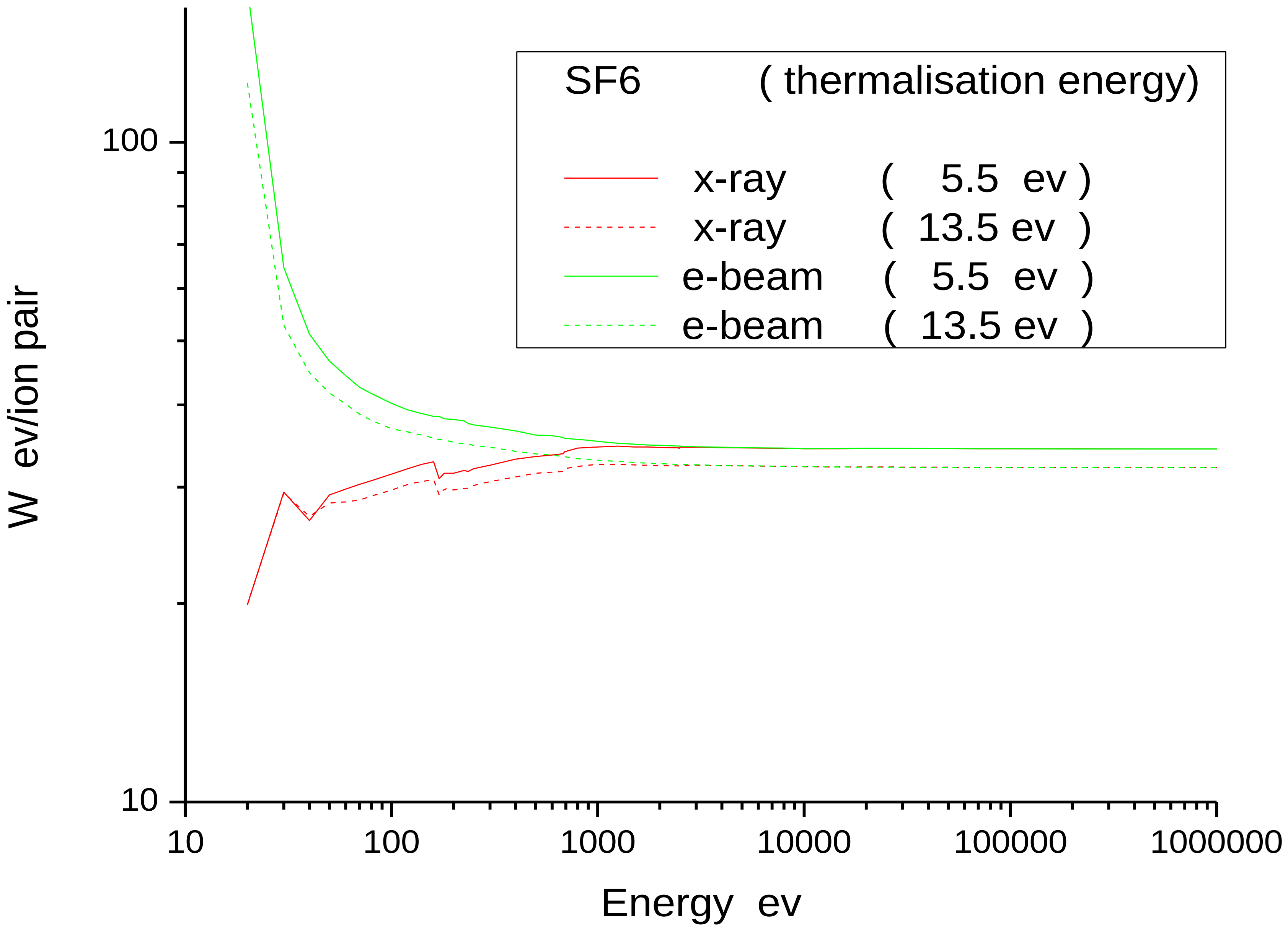


OXYGEN
R50%
R10%
R1%
Range microns
Energy ev
1E7
1000000
100000
10000
1000
100
10
1
10
100
1000
10000
100000
1000000
1E7

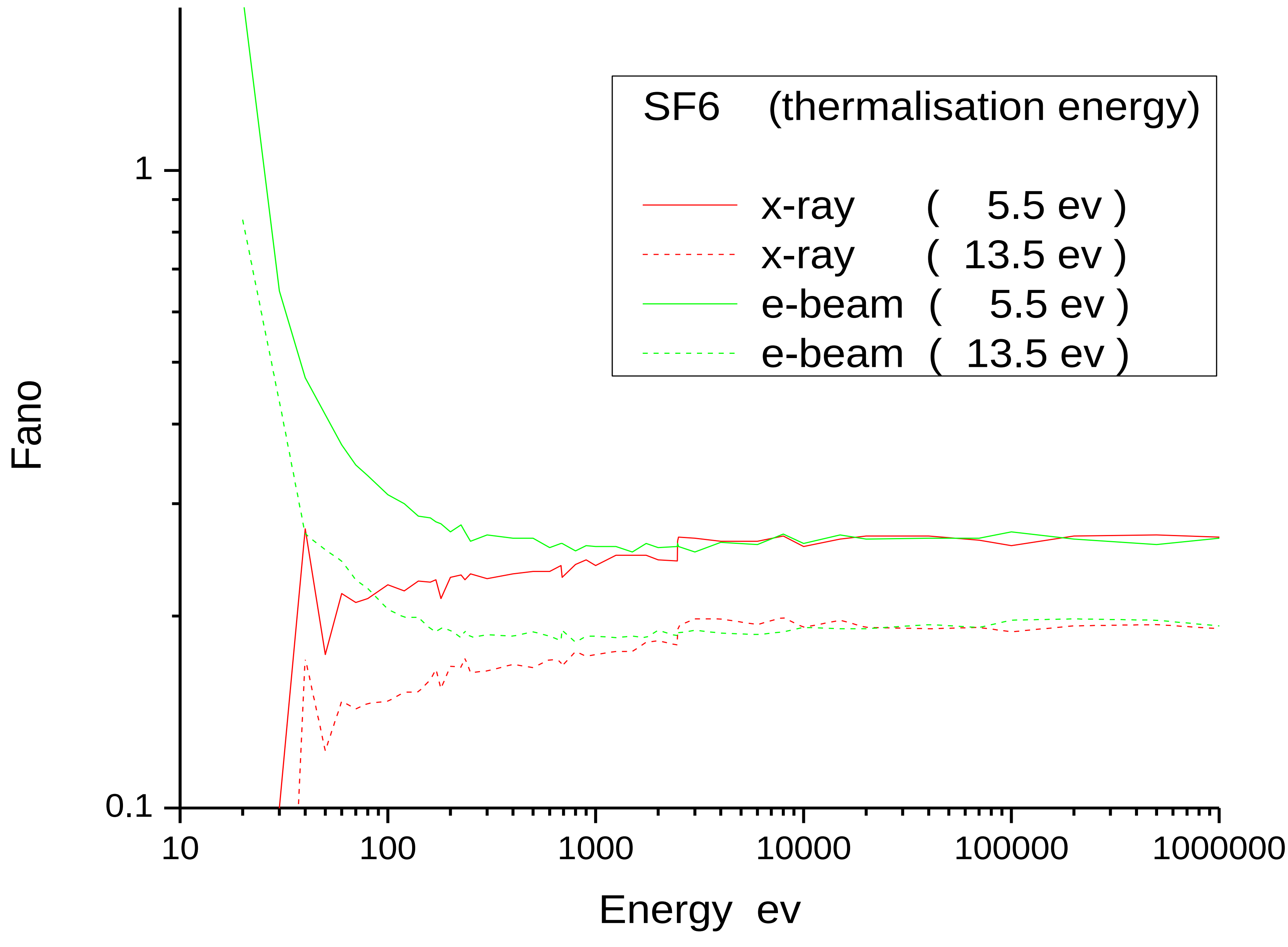

C4H10
x-ray
e-beam
W ev/ion pair
Energy ev
34
33
32
31
30
29
28
27
26
25
24
23
22
21
20
19
18
17
16
15
10
100
1000
10000
100000
1000000



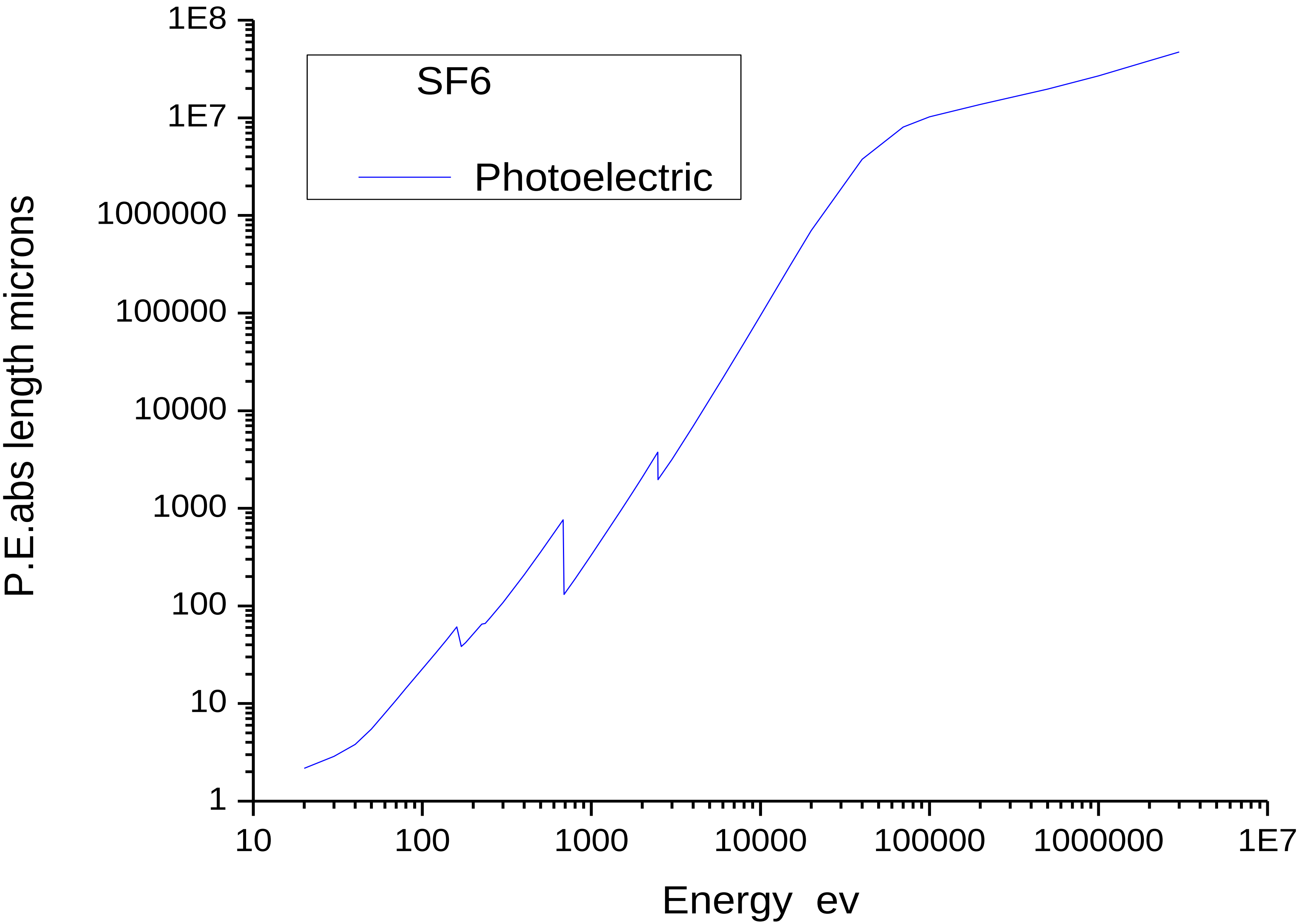
0.24
0.22
0.20
0.18
0.16
0.14
0.12
0.10
0.08
0.06
Fano
C4H10
10
100
1000
10000
100000
1000000
Energy ev

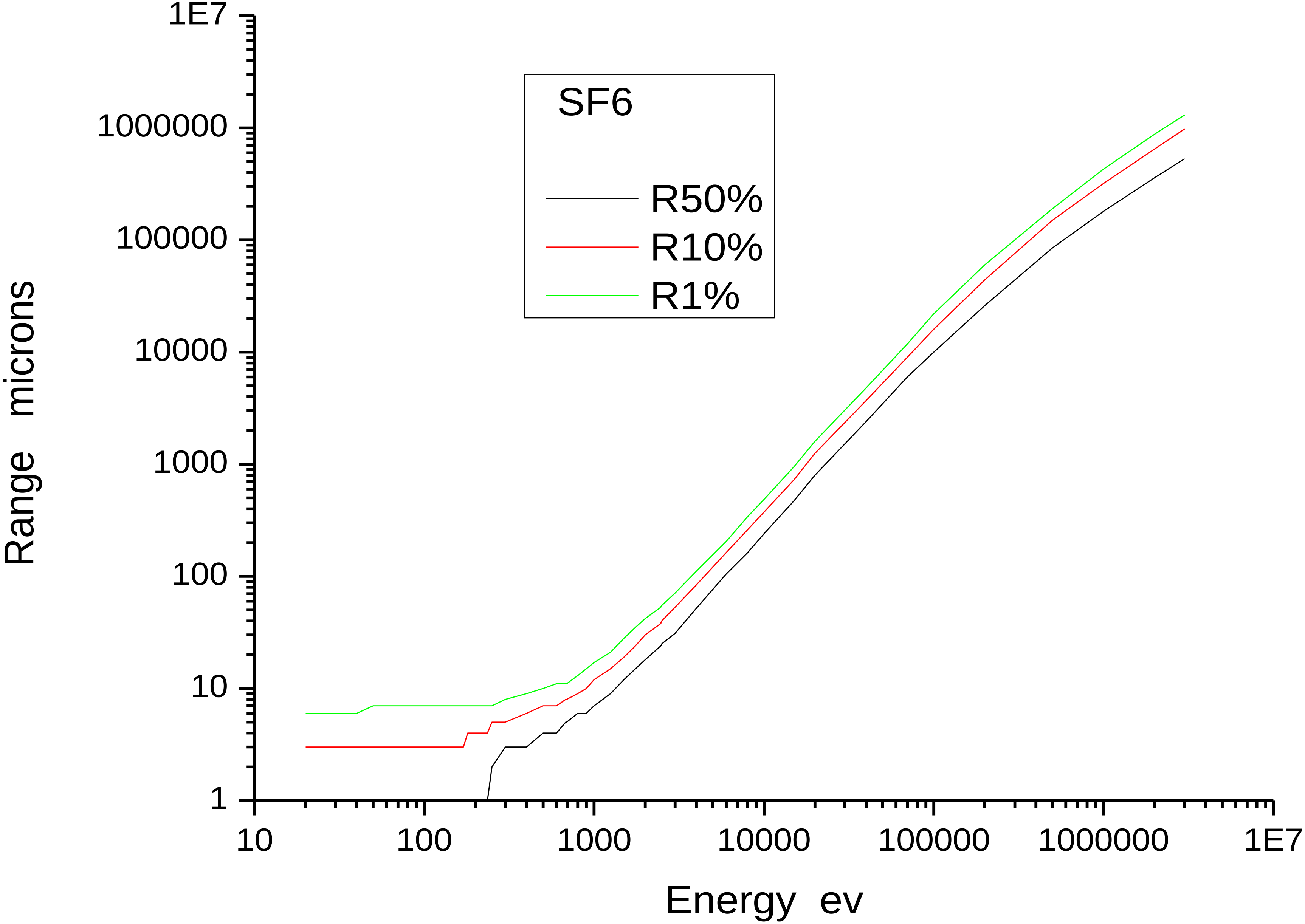


SF6 (thermalisation energy)
x-ray (5.5 ev)
x-ray (13.5 ev)
e-beam (5.5 ev)
e-beam (13.5 ev)
W ev/ion pair
100
10
10
100
1000
10000
100000
1000000
Energy ev

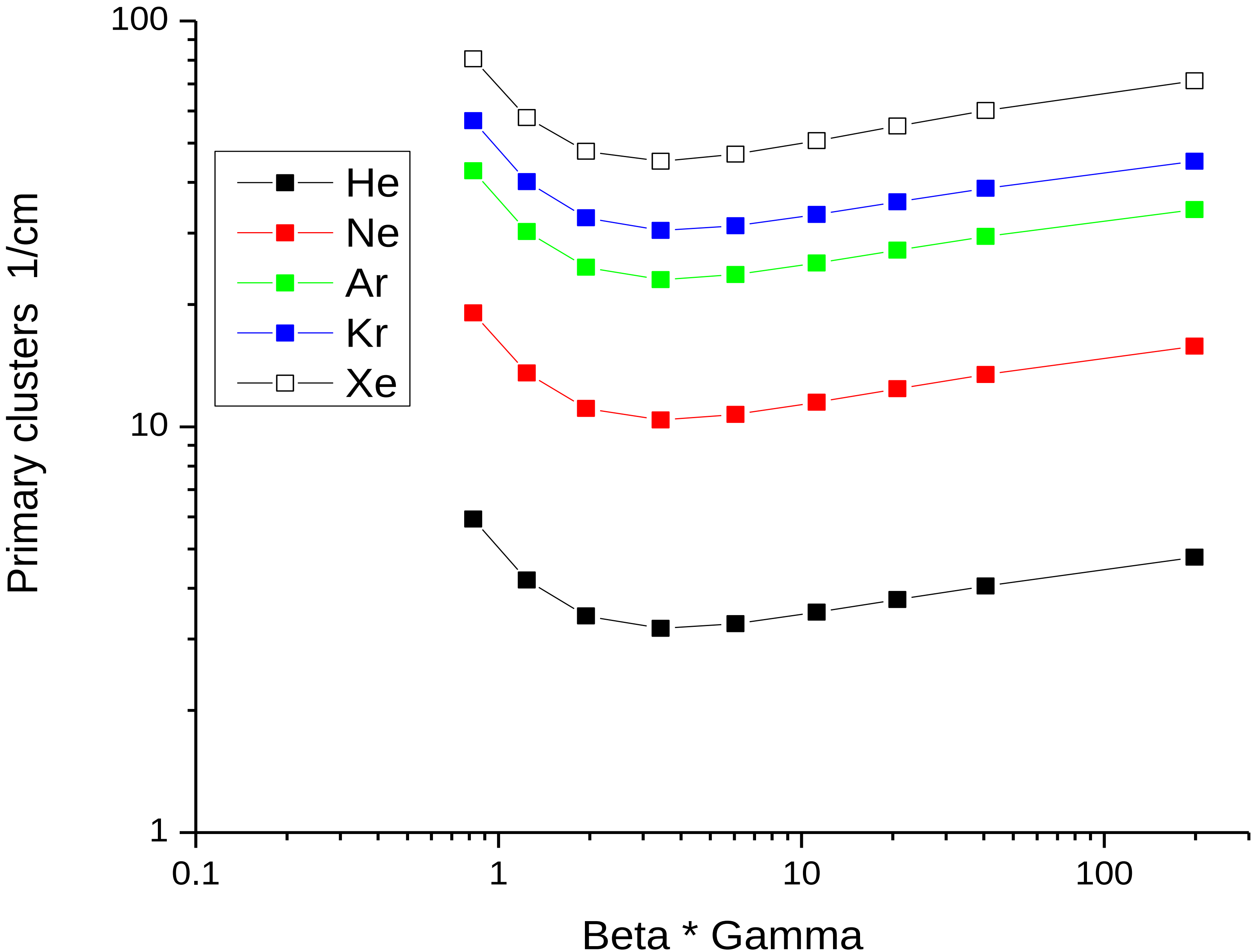


SF6 (thermalisation energy)
x-ray (5.5 ev)
x-ray (13.5 ev)
e-beam (5.5 ev)
e-beam (13.5 ev)
Fano
1
0.1
10
100
1000
10000
100000
1000000
Energy ev

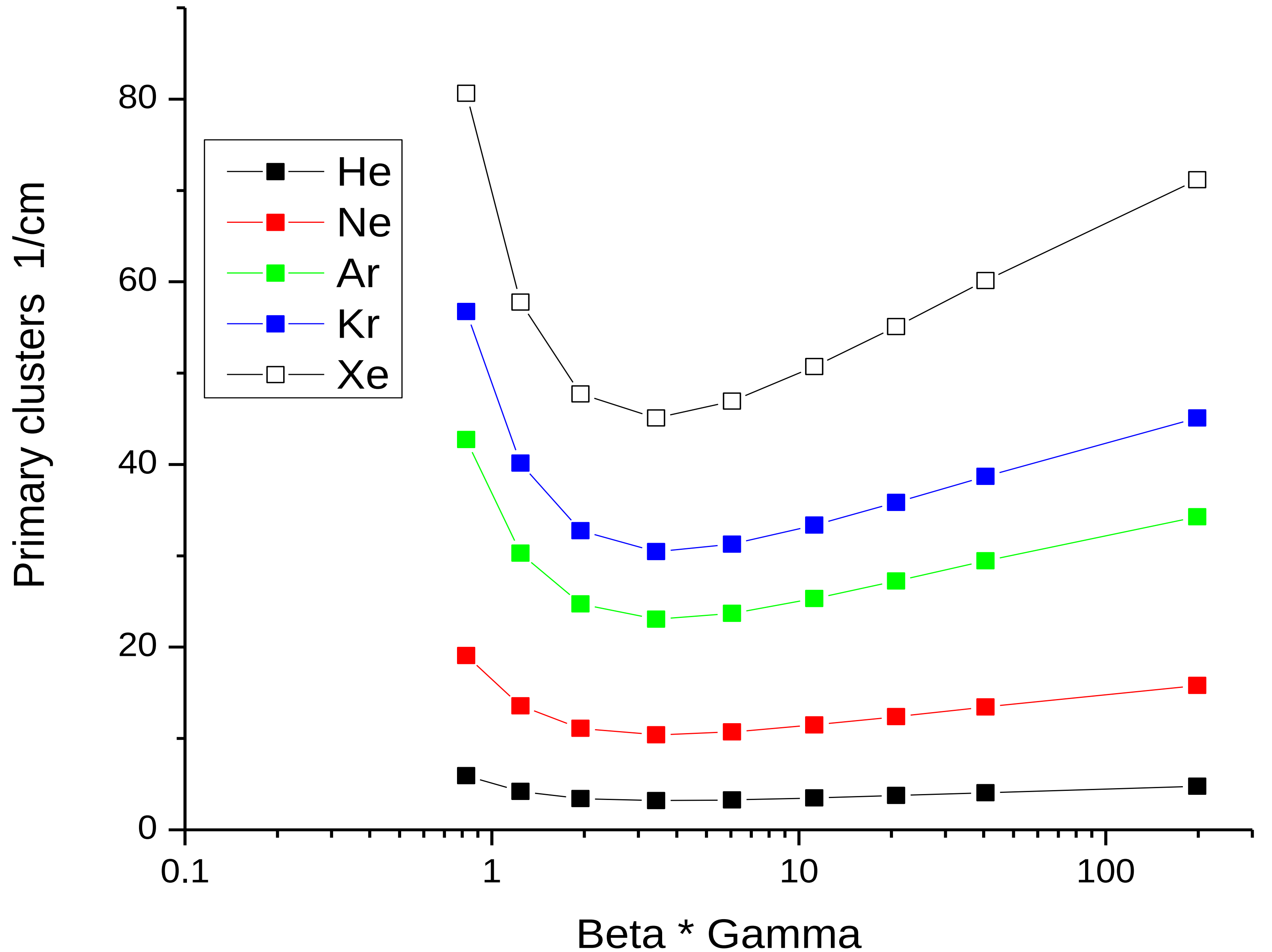

SF6
Photoelectric
P.E.abs length microns
Energy ev
1E8
1E7
1000000
100000
10000
1000
100
10
1
10
100
1000
10000
100000
1000000
1E7



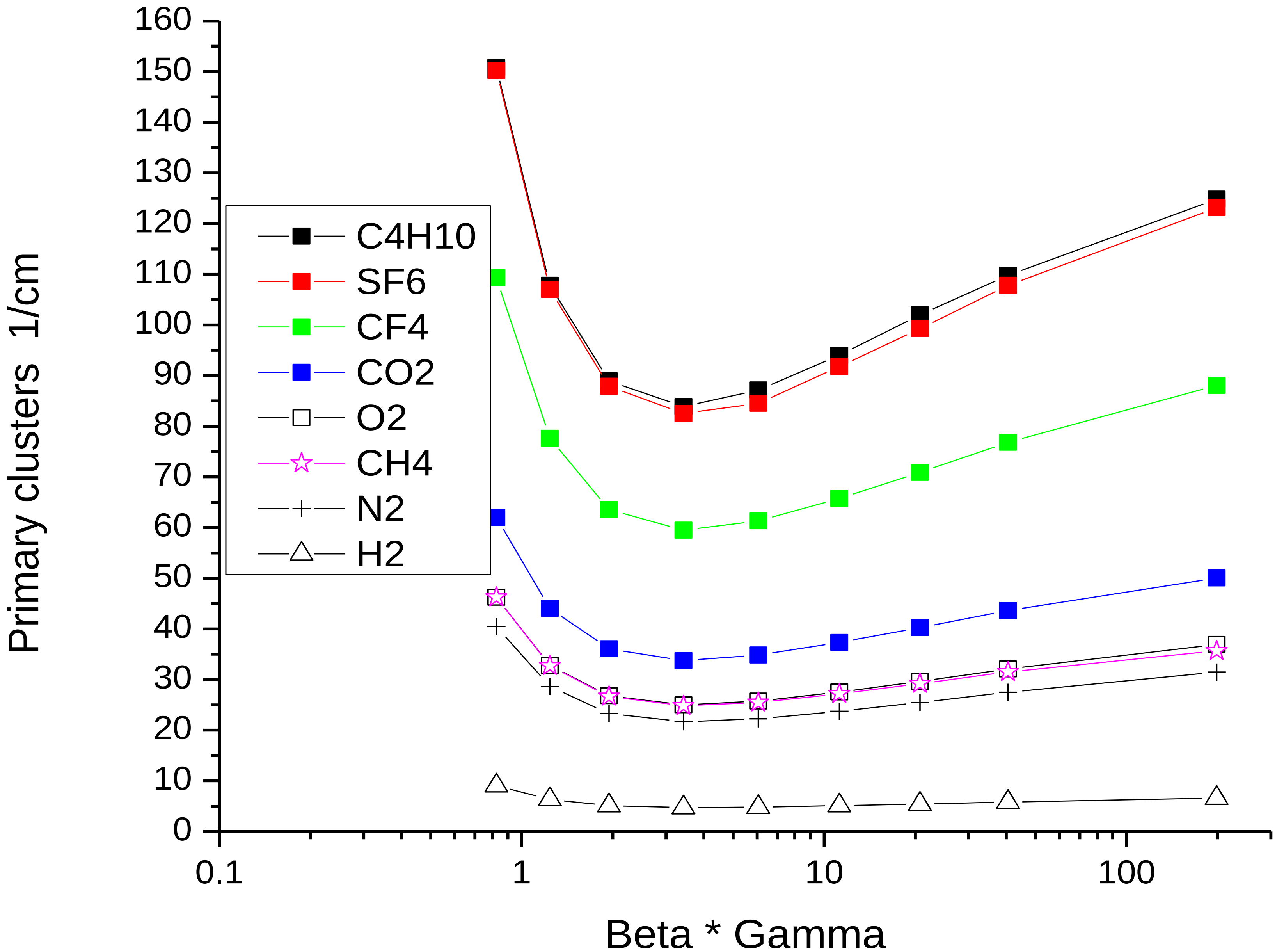
SF6
R50%
R10%
R1%
Range microns
Energy ev
1E7
1000000
100000
10000
1000
100
10
1
10
100
1000
10000
100000
1000000
1E7



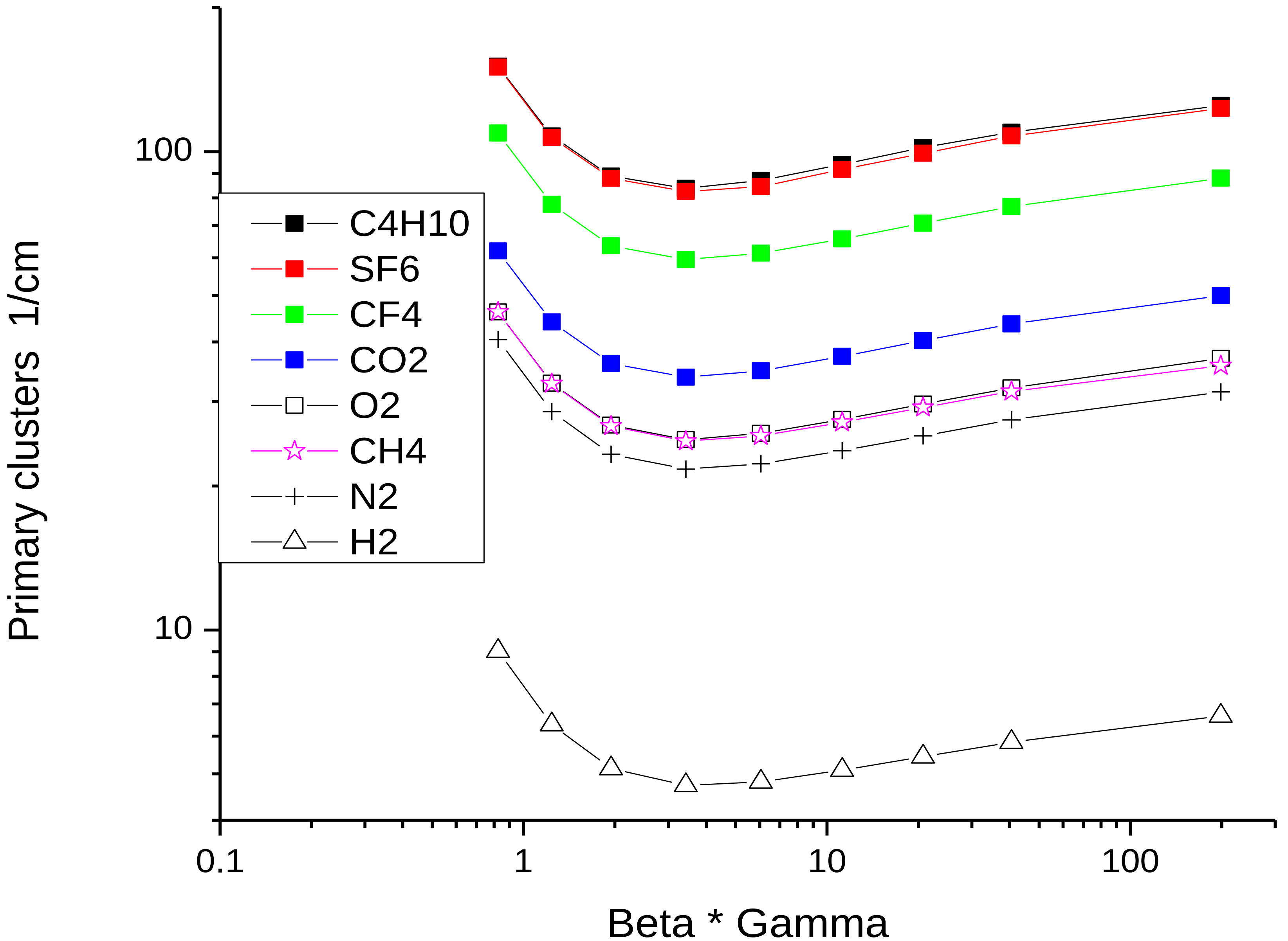
100
10
1
Primary clusters 1/cm
0.1
1
10
100
Beta * Gamma
He
Ne
Ar
Kr
Xe



Primary clusters 1/cm
Beta * Gamma
He
Ne
Ar
Kr
Xe
0
20
40
60
80
0.1
1
10
100



160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Primary clusters 1/cm
C4H10
SF6
CF4
CO2
O2
CH4
N2
H2
0.1
1
10
100
Beta * Gamma



Primary clusters 1/cm
Beta * Gamma
100
10
0.1
1
10
100
C4H10
SF6
CF4
CO2
O2
CH4
N2
H2

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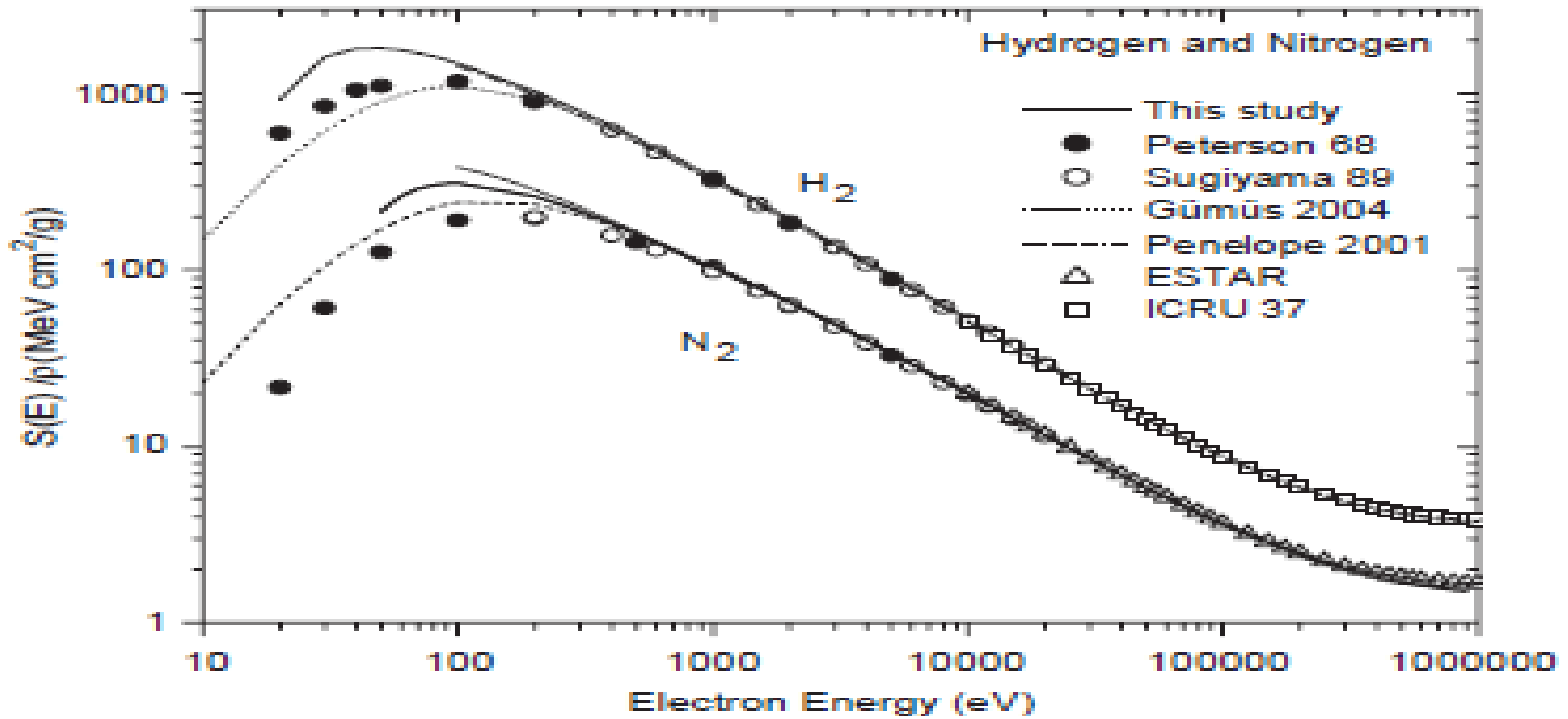
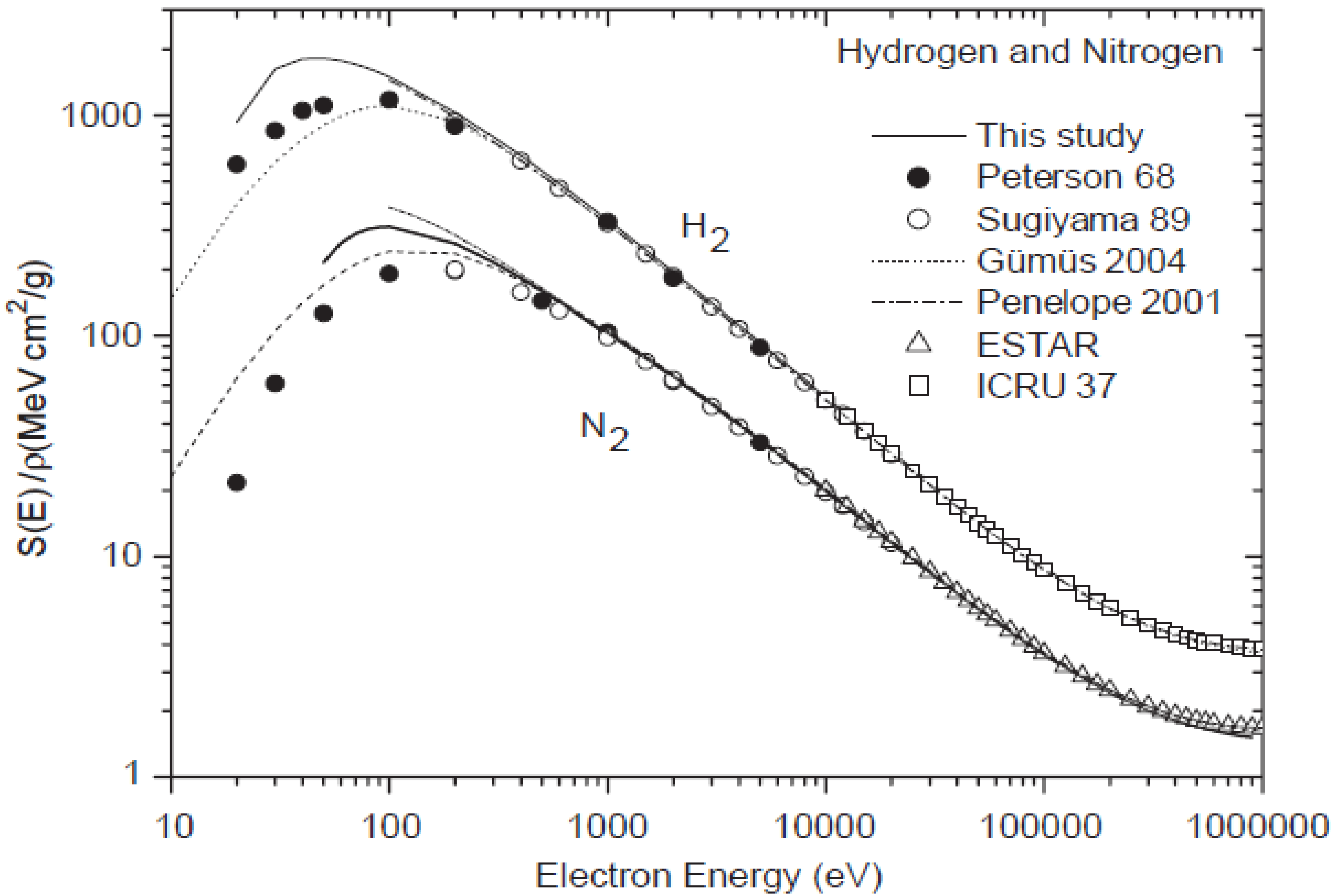
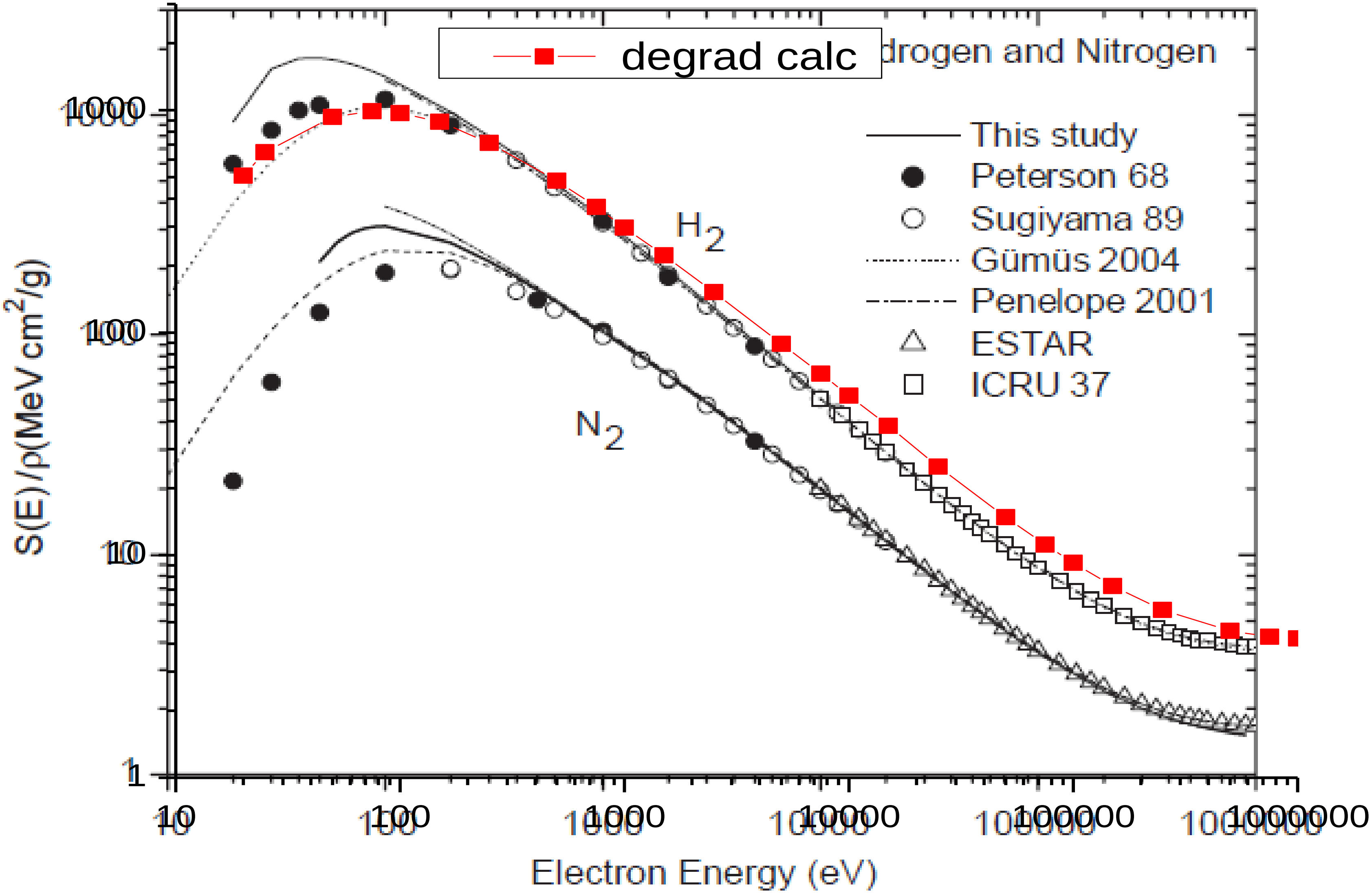
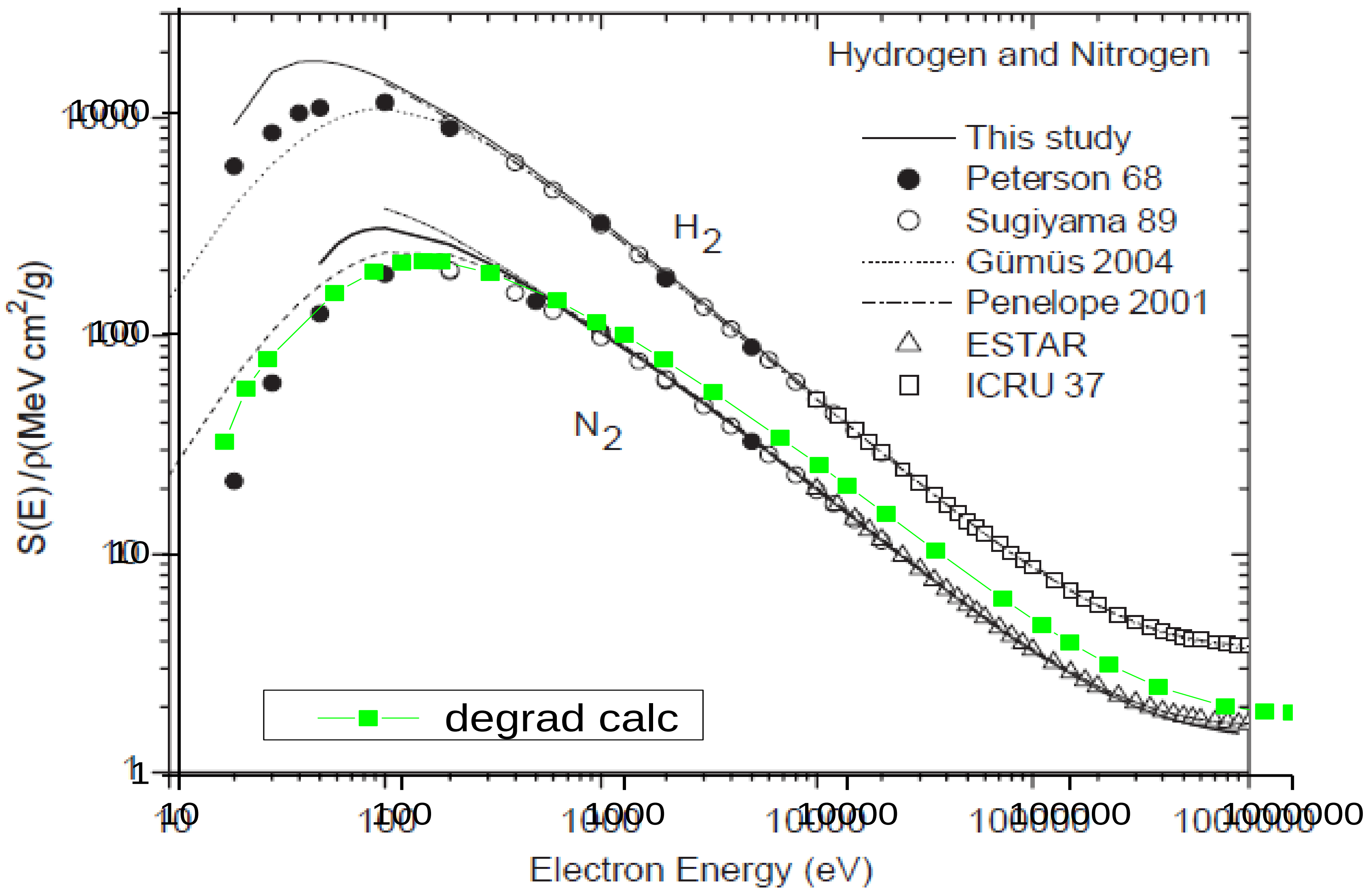


Fig. 2. Mass stopping power $S(E)/\rho$ for incident electron energies, in H_2 and N_2 targets. —, present study; ●, semiempirical formula of Peterson and Green (1968); ○, theoretical data of Sugiyama (1989); …, theoretical data of Gümüş (2005); – · –, results calculated by PENELOPE Program; △, results obtained from ESTAR (The NIST database, 2003); □, data from ICRU 37 report (1984).



Hydrogen and Nitrogen
This study
Peterson 68
Sugiyama 89
Gümüs 2004
Penelope 2001
ESTAR
ICRU 37
H2
N2
S(E)/ρ(MeV cm2/g)
Electron Energy (eV)
1000
100
10
1
10
100
1000
10000
100000
1000000


degrad calc
drogen and Nitrogen
This study
Peterson 68
Sugiyama 89
Gümüs 2004
Penelope 2001
ESTAR
ICRU 37
H2
N2
S(E)/ρ(MeV cm2/g)
Electron Energy (eV)
1
10
100
1000
10
100
1000
10000
100000
1000000



Hydrogen and Nitrogen
This study
Peterson 68
Sugiyama 89
Gümüs 2004
Penelope 2001
ESTAR
ICRU 37
H2
N2
degrad calc
S(E)/ρ(MeV cm2/g)
Electron Energy (eV)
1000
100
10
1
10
100
1000
10000
100000
1000000

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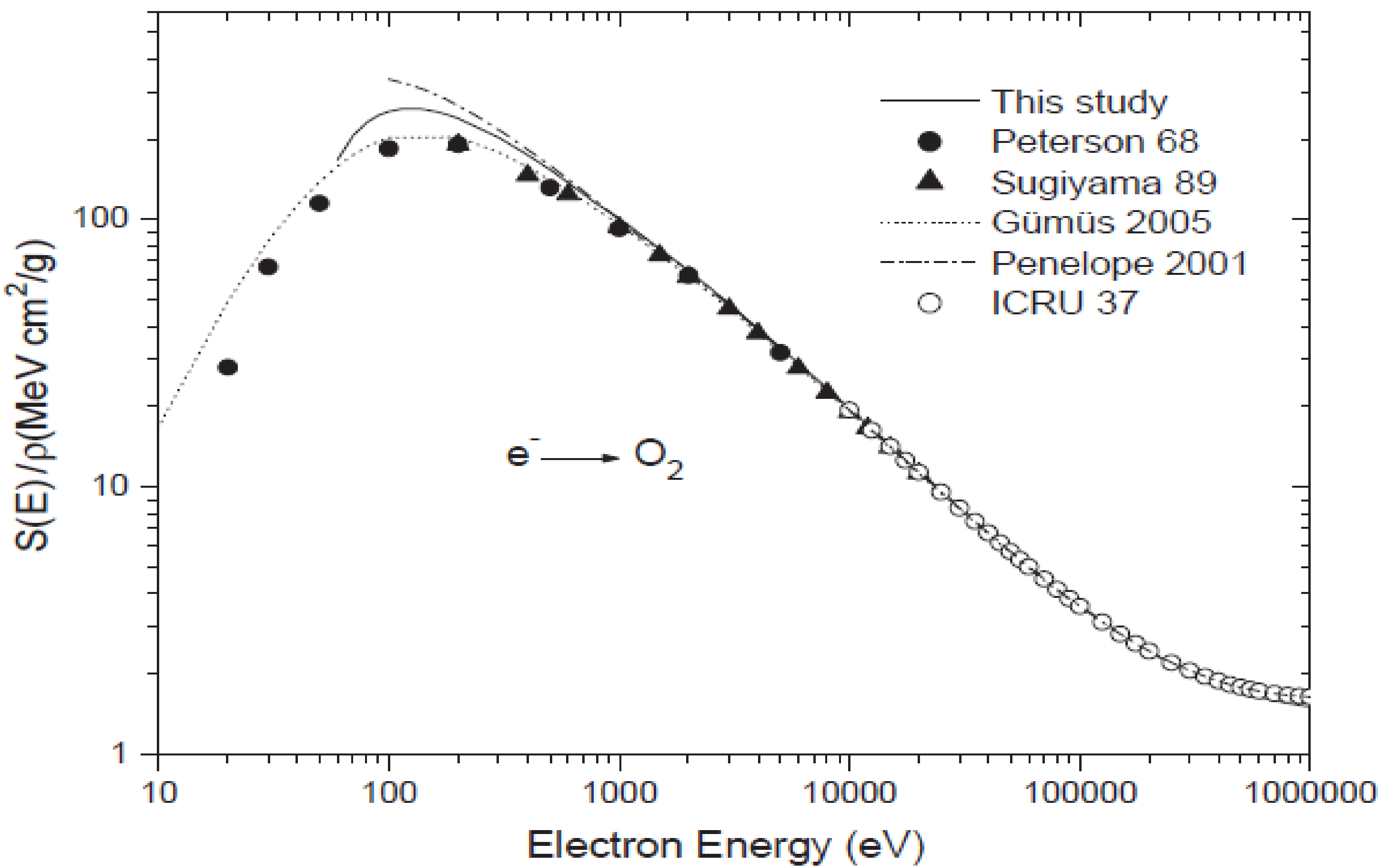

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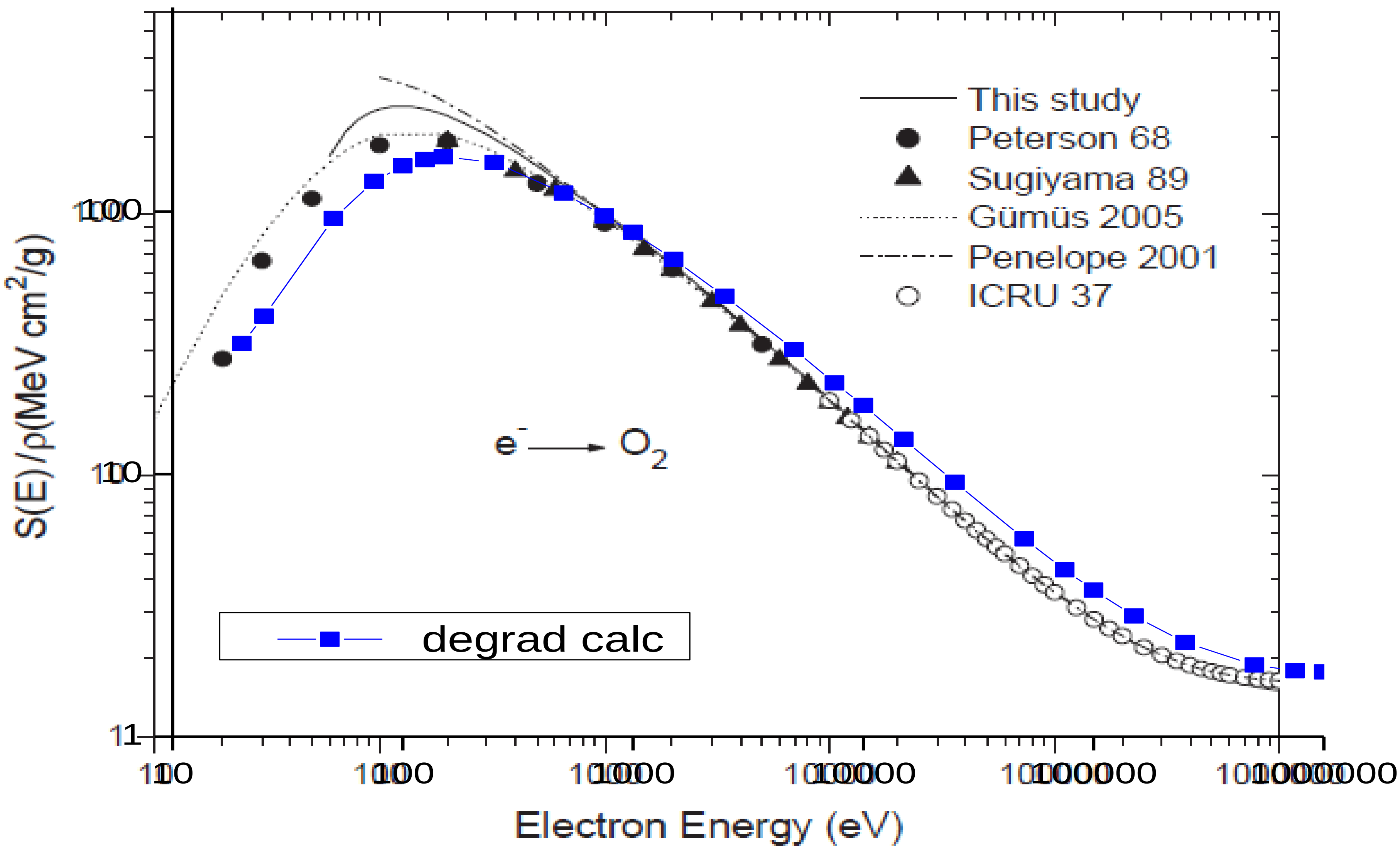

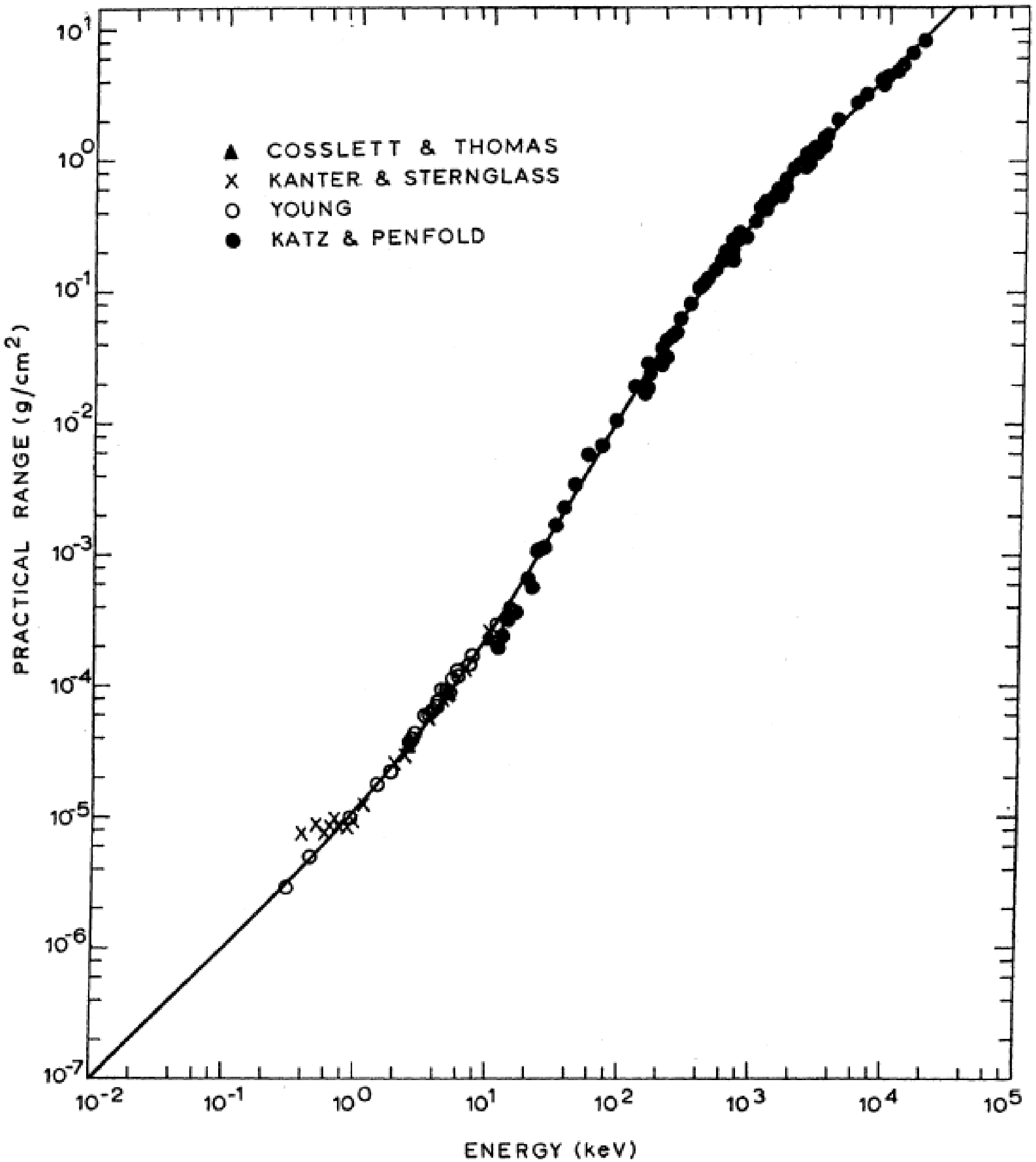
COSSLETT & THOMAS
KANTER & STERNGLASS
YOUNG
KATZ & PENFOLD
PRACTICAL RANGE (g/cm²)
ENERGY (keV)
10¹
10⁰
10⁻¹
10⁻²
10⁻³
10⁻⁴
10⁻⁵
10⁻⁶
10⁻⁷
10⁻²
10⁻¹
10⁰
10¹
10²
10³
10⁴
10⁵

Noble Gas asymptotic Fano factors

Gas	We	Fe	Wexc	Fexc	sqrt(Fe/Fexc)	experiment(icru)
He	47.1	0.235	68.8	0.68	0.59	41.3
Ne	37.4	0.135	76.8	0.68	0.44	35.4
Ar	26.3	0.144	60.1	0.71	0.45	26.4
Kr	24.8	0.158	46.8	0.72	0.47	24.4
Xe	22.3	0.181	39.4	0.76	0.49	22.1
error	1%		2%			2%

The difference between the calculation and the experiment in Helium and Neon is caused by gas impurities in the measurements which give Penning contributions to the total ionisation.

Molecular Gas asymptotic Fano factors

Gas	W	F	Wexc	Fexc	Experiment(ICRU)
CF4	28.9	0.178			
CH4	27.3	0.23			27.3
C4H10	22.2	0.124			23.4
CO2	32.9	0.239			32.8
N2	34.2	0.19			34.8
H2 min	35	0.28	28.6	0.53	36.5
H2 max	36.8	0.46	27.1	0.67	36.5
O2	29.2	0.18			30.5
O2-3B	30.1	0.19			30.5
TMA	15	0.14			
SF6	32.2-34.3	0.2-0.265			33.8
error	2%		3%		2%

Comments: Hydrogen has a large rise from the minimum at about 1Kev to a Maximum at 1Mev so the two values are given in the table , the other gases display a rise of less than 1% from the minimum to maximum at high energy .

C4H10 has low F (no data on dissociative ionisation)

O2-3B includes effect of 3 body attachment on W and F

SF6 values at 13 ev and 5.5 ev thermalisation energy (5.5ev typical for RPC)

Charged particle track cluster size distribution for Noble gases

Cluster Size	He	Ne	Ar	Kr	Xe
1	82.1	68.8	67.8	64.4	57.4
2	9.57	15.3	13.7	14.5	16.4
3	3.07	5.41	4.88	6.02	8.79
4	1.45	2.64	2.27	3.25	4.65
5	0.828	1.54	1.28	2.01	2.62
6	0.536	1	0.813	1.32	1.62
7	0.364	0.718	0.568	0.968	1.06
8	0.287	0.547	0.466	0.76	0.791
9	0.217	0.396	0.532	0.652	0.578
10	0.164	0.311	0.681	0.538	0.448
11	0.135	0.252	0.804	0.477	0.367
12	0.121	0.206	0.781	0.419	0.297
13	0.103	0.173	0.682	0.384	0.255
14	0.08	0.155	0.563	0.321	0.204
15	0.07	0.13	0.455	0.271	0.177
16	0.059	0.116	0.379	0.251	0.148
17	0.052	0.1	0.315	0.22	0.143
18	0.04	0.091	0.265	0.194	0.117
19	0.04	0.081	0.217	0.173	0.094
20	0.038	0.072	0.185	0.147	0.09
21		0.073			
22		0.075			
23		0.08			
24		0.08			
25		0.074			
26		0.071			
>20	0.638	1.97	2.3	2.71	3.8
Shell		K	L3,L2,L1	M5 to M1	N1

Charged particle track cluster size distribution for molecular gases

Cluster size	CF4	CH4	C4H10	CO2	N2	H2	O2	SF6
1	70.5	81.4	79.9	71.4	71.3	84.3	69.3	64.5
2	14.4	9.59	9.72	14.6	14.9	8.43	15.7	16
3	5.23	3	3.45	4.61	4.44	2.66	5.19	6.19
4	2.47	1.41	1.65	2.15	2.05	1.26	2.34	3.04
5	1.41	0.793	0.939	1.26	1.18	0.73	1.38	1.78
6	0.914	0.508	0.598	0.83	0.79	0.465	0.89	1.22
7	0.616	0.347	0.404	0.61	0.56	0.334	0.62	0.99
8	0.464	0.252	0.299	0.54	0.415	0.245	0.45	0.79
9	0.35	0.207	0.222	0.49	0.336	0.198	0.37	0.66
10	0.281	0.185	0.189	0.44	0.353	0.16	0.28	0.54
11	0.254	0.171	0.161	0.325	0.463	0.12	0.23	0.45
12	0.211	0.182	0.147	0.241	0.553	0.097	0.19	0.36
13	0.181	0.165	0.148	0.192	0.532	0.089	0.17	0.296
14	0.167	0.155	0.146	0.194	0.386	0.071	0.148	0.25
15	0.147	0.136	0.144	0.217	0.232	0.06	0.127	0.211
16	0.128	0.122	0.132	0.228	0.142	0.055	0.141	0.183
17	0.108	0.105	0.126	0.221	0.1	0.049	0.177	0.173
18	0.097	0.091	0.111	0.19	0.086	0.041	0.244	0.142
19	0.087	0.079	0.095	0.139	0.077	0.035	0.299	0.136
20	0.08	0.071	0.089	0.097	0.068	0.034	0.289	0.119
>20	1.9	0.99	1.29	1.03	1	0.57	1.45	1.96
Shell	C K	C K	C K	C K O K	N K		OK	S L12 S L3
								F K

Helium De/Dx and primary cluster density

Energy Mev	0.15	0.3	0.6	1.3	2.6	5.2	10	20	100
Beta*Gamma	0.825	1.24	1.944	3.427	6.057	11.23	20.74	40.52	198.6
Np 1/cm	5.923	4.192	3.419	3.184	3.27	3.49	3.751	4.052	4.767
De/Dx elastic	0.058	0.042	0.036	0.036	0.038	0.04	0.041	0.041	0.039
De/Dx exc	58.38	41.56	34.13	32.1	33.34	35.99	39.08	42.62	51.04
De/Dx ion	478.1	353.2	299.8	290.5	308	337.8	371	408.1	492.9
De/Dx brem	0.231	0.308	0.443	0.919	2.109	4.891	11.01	25.21	155
De/Dx tot	536.8	395.1	334.4	323.5	343.4	378.7	421.1	476	699
De/Dx cut(9kev)	421	298	243	226	232	248	266	288	339
% pass cut	99.8	99.8	99.8	99.8	99.8	99.8	99.8	99.8	99.8

Minimum ionising (without brem) : Estar =295.7

Groom =322.2

Degrad =322.6

Neon De/Dx and primary cluster density

Energy Mev	0.15	0.3	0.6	1.3	2.6	5.2	10	20	100
Beta*Gamma	0.825	1.24	1.944	3.427	6.057	11.23	20.74	40.52	198.6
Np 1/cm	19.08	13.56	11.1	10.39	10.72	11.49	12.4	13.44	15.8
De/Dx elastic	0.27	0.2	0.17	0.17	0.18	0.19	0.2	0.2	0.19
De/Dx exc	40.69	28.96	23.77	22.35	23.19	25	27.12	29.54	35.05
De/Dx ion	2251	1693	1462	1444	1558	1737	1936	2162	2680
De/Dx brem	5.686	7.102	9.499	18.37	39.98	89.08	194.2	432.8	2553
De/Dx tot	2297	1729	1496	1485	1621	1851	2157	2625	5269
De/Dx cut(9kev)	1896	1352	1111	1043	1080	1161	1256	1365	1613
% pass cut	99.1	99	99	99	99	99	99	99	99

Minimum ionising (without brem) : Estar =1313
Groom =1446
Degrad =1467

Argon De/Dx and primary cluster density

Energy Mev	0.15	0.3	0.6	1.3	2.6	5.2	10	20	100
Beta*Gamma	0.825	1.24	1.944	3.427	6.057	11.23	20.74	40.52	198.6
Np 1/cm	42.73	30.28	24.72	23.05	23.71	25.33	27.25	29.46	34.27
De/Dx elastic	0.42	0.31	0.27	0.27	0.29	0.3	0.31	0.32	0.3
De/Dx exc	123.6	87.99	72.24	67.85	70.31	75.69	81.97	89.17	104.8
De/Dx ion	4278	3216	2770	2736	2948	3288	3668	4104	5134
De/Dx brem	19.47	24.01	31.24	58.92	125.3	275.3	592	1304	7629
De/Dx tot	4422	3328	2874	2863	3144	3639	4342	5497	12870
De/Dx cut(9kev)	3635	2598	2137	2013	2087	2248	2435	2650	3139
% pass cut	97.3	97.2	97.1	97	97	97.1	97.1	97.1	97.1

Minimum ionising (without brem) : Estar = 2297
Groom = 2452
Degrad = 2805

Krypton De/Dx and primary cluster density

Energy Mev	0.15	0.3	0.6	1.3	2.6	5.2	10	20	100
Beta*Gamma	0.825	1.24	1.944	3.427	6.057	11.23	20.74	40.52	198.6
Np 1/cm	56.75	40.15	32.74	30.46	31.27	33.36	35.84	38.7	45.08
De/Dx elastic	0.8	0.61	0.54	0.53	0.56	0.6	0.61	0.63	0.57
De/Dx exc	161.3	114.7	94.12	88.31	91.41	98.3	106.4	115.6	136.3
De/Dx ion	6736	5152	4510	4516	4929	5560	6266	7077	9053
De/Dx brem	84.24	104.9	133.8	243	495.9	1059	2226	4833	27780
De/Dx tot	6982	5373	4739	4848	5517	6718	8599	12030	36970
De/Dx cut(9kev)	5255	3744	3071	2879	2975	3194	3451	3744	4419
% pass cut	87	86.8	86.7	86.6	86.6	86.6	86.6	86.6	86.6

Minimum ionising (without brem) : Estar = 4254
Groom = 4731
Degrad = 4605

Xenon De/Dx and primary cluster density

Energy Mev	0.15	0.3	0.6	1.3	2.6	5.2	10	20	100
Beta*Gamma	0.825	1.24	1.944	3.427	6.057	11.23	20.74	40.52	198.6
Np 1/cm	80.63	57.76	47.71	45.08	46.93	50.72	55.1	60.13	71.17
De/Dx elastic	1.15	0.9	0.8	0.79	0.84	0.89	0.91	0.92	0.96
De/Dx exc	204.3	145.4	119.2	111.8	115.7	124.4	134.5	146.2	171.9
De/Dx ion	10110	7822	6928	7030	7761	8848	10070	11470	14920
De/Dx brem	91.75	163.2	279	565.2	1153	2394	4926	10470	58850
De/Dx tot	10410	8131	7327	7708	9030	11370	15130	22090	73940
De/Dx cut(9kev)	7890	5699	4746	4524	4747	5167	5653	6198	7453
% pass cut	77.4	77.1	76.9	76.8	76.8	76.8	76.8	76.8	76.7

Minimum ionising (without brem) : Estar = 6146
Groom = 6882
Degrad = 7143

CF_4 De/Dx and primary cluster density

Energy Mev	0.15	0.3	0.6	1.3	2.6	5.2	10	20	100
Beta*Gamma	0.825	1.24	1.944	3.427	6.057	11.23	20.74	40.52	198.6
Np 1/cm	109.3	77.63	63.56	59.46	61.33	65.72	70.88	76.81	88.06
De/Dx elastic	0.221	0.163	0.14	0.141	0.148	0.157	0.162	0.166	0.161
De/Dx exc	169.1	120.8	99.51	93.7	97.3	104.8	113.6	123.7	142.7
De/Dx ion	9829	7380	6356	6270	6753	7527	8397	9398	11560
De/Dx brem	19.79	24.82	33.41	64.96	141.8	318.2	696.2	1555	9197
De/Dx tot	10020	7526	6489	6429	6993	7950	9207	11080	20900
De/Dx cut(9kev)	8344	5950	4887	4592	4754	5113	5531	6012	6970
% pass cut	99.6	99.5	99.5	99.5	99.5	99.5	99.5	99.5	99.5

Minimum ionising (without brem) : Groom =6382
Degrad =6364

CH4 De/Dx and primary cluster density

Energy Mev	0.15	0.3	0.6	1.3	2.6	5.2	10	20	100
Beta*Gamma	0.825	1.24	1.944	3.427	6.057	11.23	20.74	40.52	198.6
Np 1/cm	46.23	32.71	26.67	24.81	25.47	27.17	29.19	31.52	35.68
De/Dx elastic	0.135	0.098	0.084	0.083	0.088	0.093	0.097	0.099	0.097
De/Dx exc	294.3	209.6	172.1	161.6	167.4	180.1	195	212.1	242.6
De/Dx ion	2583	1914	1627	1584	1685	1858	2053	2277	2743
De/Dx brem	2251	2.89	3.992	7.968	17.8	40.61	90.08	204	1237
De/Dx tot	2880	2127	1803	1753	1871	2079	2338	2693	4223
De/Dx cut(9kev)	2265	1607	1312	1225	1261	1349	1453	1573	1799
% pass cut	99.9	99.8	99.8	99.8	99.8	99.8	99.8	99.8	99.8

Minimum ionising (without brem) : Estar = 1479
Groom = 1613
Degrad = 1745

C4H10 De/Dx and primary cluster density

Energy Mev	0.15	0.3	0.6	1.3	2.6	5.2	10	20	100
Beta*Gamma	0.825	1.24	1.944	3.427	6.057	11.23	20.74	40.52	198.6
Np 1/cm	150.8	107.8	88.92	83.85	87.13	94.01	102	109.8	124.8
De/Dx elastic	0.143	0.105	0.089	0.09	0.095	0.101	0.103	0.106	0.105
De/Dx exc	219.9	156.7	128.7	120.8	125.1	134.4	145.4	156.2	176.8
De/Dx ion	8632	6458	5542	5456	5865	6527	7264	8043	9748
De/Dx brem	8.6	11.1	15.2	30.2	67.2	153	339	765	4623
De/Dx tot	8861	6626	5686	5607	6057	6814	7749	8965	14550
De/Dx cut(9kev)	7564	5418	4466	4221	4390	4744	5152	5568	6398
% pass cut	99.8	99.6	99.6	99.6	99.6	99.6	99.6	99.6	99.6

Minimum ionising (without brem) : Estar = 5110
Groom = 5670
Degrad = 5577

CO_2 De/Dx and primary cluster density

Energy Mev	0.15	0.3	0.6	1.3	2.6	5.2	10	20	100
Beta*Gamma	0.825	1.24	1.944	3.427	6.057	11.23	20.74	40.52	198.6
Np 1/cm	61.97	44.04	36.07	33.75	34.82	37.32	40.26	43.63	50.03
De/Dx elastic	0.199	0.146	0.126	0.125	0.132	0.14	0.146	0.149	0.146
De/Dx exc	240	169	138	129	133	143	154	168	193
De/Dx ion	5313	3956	3382	3309	3541	3924	4356	4850	5870
De/Dx brem	8.979	11.33	15.32	29.95	65.76	148.1	324.6	727.6	4333
De/Dx tot	5561	4136	3536	3468	3740	4215	4835	5746	10400
De/Dx cut(9kev)	4630	3294	2702	2533	2617	2809	3035	3293	3796
% pass cut	99.9	99.9	99.9	99.9	99.9	99.9	99.9	99.9	99.9

Minimum ionising (without brem) : Estar = 3053
Groom = 3351
Degrad = 3438

N2 De/Dx and primary cluster density

Energy Mev	0.15	0.3	0.6	1.3	2.6	5.2	10	20	100
Beta*Gamma	0.825	1.24	1.944	3.427	6.057	11.23	20.74	40.52	198.6
Np 1/cm	40.46	28.61	23.31	21.68	22.24	23.71	25.46	27.48	31.47
De/Dx elastic	0.19	0.139	0.119	0.12	0.127	0.134	0.138	0.142	0.138
De/Dx exc	214.7	153.3	126.1	118.7	123.2	132.7	143.7	156.4	181.5
De/Dx ion	3491	2584	2197	2135	2272	2505	2771	3078	3760
De/Dx brem	5.481	6.924	9.388	18.4	40.52	91.26	201	450.5	2693
De/Dx tot	3711	2745	2333	2272	2435	2729	3116	3685	6614
De/Dx cut(9kev)	3053	2163	1765	1646	1692	1807	1944	2101	2420
% pass cut	99.9	99.9	99.9	99.9	99.9	99.9	99.9	99.9	99.9

Minimum ionising (without brem) : Estar = 1947
Groom = 2127
Degrad = 2254

H2 De/Dx and primary cluster density

Energy Mev	0.15	0.3	0.6	1.3	2.6	5.2	10	20	100
Beta*Gamma	0.825	1.24	1.944	3.427	6.057	11.23	20.74	40.52	198.6
Np 1/cm	9.026	6.339	5.129	4.729	4.813	5.092	5.432	5.826	6.611
De/Dx elastic	0.06	0.043	0.037	0.036	0.037	0.04	0.04	0.041	0.038
De/Dx exc	134.5	95.99	78.99	74.31	77.06	82.98	89.87	97.75	113.4
De/Dx ion	474.4	347	291.5	278.9	292.2	316.8	344.4	375.2	435.3
De/Dx brem	0.126	0.176	0.266	0.578	1.368	3.263	7.483	17.46	112.1
De/Dx tot	609	443.2	370.8	353.8	370.7	403.1	441.8	490.4	660.9
De/Dx cut(9kev)	420.8	295.4	239.1	220.4	224.3	237.2	253.1	271.4	308
% pass cut	99.9	99.9	99.9	99.9	99.9	99.9	99.9	99.9	99.9

Minimum ionising (without brem) : Estar = 317.4
Groom = 343.7
Degrad = 353.2

O2 De/Dx and primary cluster density

Energy Mev	0.15	0.3	0.6	1.3	2.6	5.2	10	20	100
Beta*Gamma	0.825	1.24	1.944	3.427	6.057	11.23	20.74	40.52	198.6
Np 1/cm	46.23	32.78	26.8	25.01	25.75	27.54	29.65	32.08	36.95
De/Dx elastic	0.217	0.159	0.137	0.137	0.145	0.153	0.158	0.162	0.157
De/Dx exc	80.08	56.72	46.35	43.36	44.82	48.17	52.12	56.66	65.76
De/Dx ion	3757	2790	2380	2322	2479	2740	3035	3372	4085
De/Dx brem	7.19	9.05	12.2	23.79	52.18	117.3	256.9	575.4	3420
De/Dx tot	3844	2856	2439	2390	2576	2906	3344	4004	7571
De/Dx cut(9kev)	3283	2332	1909	1786	1841	1973	2128	2305	2667
% pass cut	99.94	99.94	99.94	99.93	99.93	99.93	99.93	99.93	99.93

Minimum ionising (without brem) : Estar = 2185
Groom = 2373
Degrad = 2366

SF6 De/Dx and primary cluster density

Energy Mev	0.15	0.3	0.6	1.3	2.6	5.2	10	20	100
Beta*Gamma	0.825	1.24	1.944	3.427	6.057	11.23	20.74	40.52	198.6
Np 1/cm	150.2	107	87.91	82.53	84.51	91.79	99.26	107.8	123.1
De/Dx elastic	0.269	0.199	0.172	0.171	0.18	0.19	0.198	0.204	0.196
De/Dx exc	298.4	213.1	175.5	165.2	171.4	184.7	200.1	217.7	249.4
De/Dx ion	17300	13070	11330	11240	12180	13650	15300	17190	21180
De/Dx brem	41.85	52.12	69.4	133.7	289.4	645.2	1404	3120	18390
De/Dx tot	17640	13330	11570	11540	12640	14480	16900	20530	39820
De/Dx cut(9kev)	14440	10310	8482	7982	8278	8916	9659	10510	12120
% pass cut	97.7	97.6	97.5	97.5	97.5	97.4	97.4	97.4	97.4

Minimum ionising (without brem) : Estar =

Groom =

Degrad = 11406

Conclusion:

Many thanks to Carlos Oliveira and Carlos Azevado whose help in debugging Degrad was essential to finishing this project.

The data base now covers the most important gases used in radiation detectors with more than adequate precision .

The next priorities for the future include the addition of x-sections for liquid argon and xenon thanks to the work of ANU and James Cook University Australia (Ron White) .

The priorities after that will be to upgrade H2O and propane to be included in degrad so as to allow better simulation of tissue equivalent gases for radiation damage simulation of biological structures..

Liquid Argon and Xenon:

20 years ago I simulated the behaviour of liquids using some x-sections close to those of Lekner. The aim was to see the effect of doping liquid Argon with Methane which was used at that Time for speeding up the response of electromagnetic calorimeters.

The calculated drift velocity increase with doping was roughly comparable with that obtained in experiment. However the accuracy of the simulation did not warrant publication at that time.

Recently Ron White published a new analysis and cross-sections for Liquid Argon ref J.Chem.Phys 142(2015)154507

the paper had a much better treatment of liquid state than in the Lekner theory in particular the pair structure factor and reproduces drift velocity and diffusion accurately.

I e-mailed Ron and asked if it was possible to do the same for Xenon and he has sent a preprint which I can not yet make public But hopefully will soon be published in NIMA..

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Electron scattering and transport in liquid argon

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The transport of excess electrons in liquid argon driven out of equilibrium by an applied electric field is revisited using a multi-term solution of Boltzmann's equation together with *ab initio* liquid phase cross-sections calculated using the Dirac-Fock scattering equations. The calculation of liquid phase cross-sections extends previous treatments to consider multipole polarisabilities and a non-local treatment of exchange, while the accuracy of the electron-argon potential is validated through comparison of the calculated gas phase cross-sections with experiment. The results presented highlight the inadequacy of local treatments of exchange that are commonly used in liquid and cluster phase cross-section calculations. The multi-term Boltzmann equation framework accounting for coherent scattering enables the inclusion of the full anisotropy in the differential cross-section arising from the interaction and the structure factor, without an *a priori* assumption of quasi-isotropy in the velocity distribution function. The model, which contains no free parameters and accounts for both coherent scattering and liquid phase screening effects, was found to reproduce well the experimental drift velocities and characteristic energies. © *2015 AIP Publishing LLC.* [http://dx.doi.org/10.1063/1.4917258]

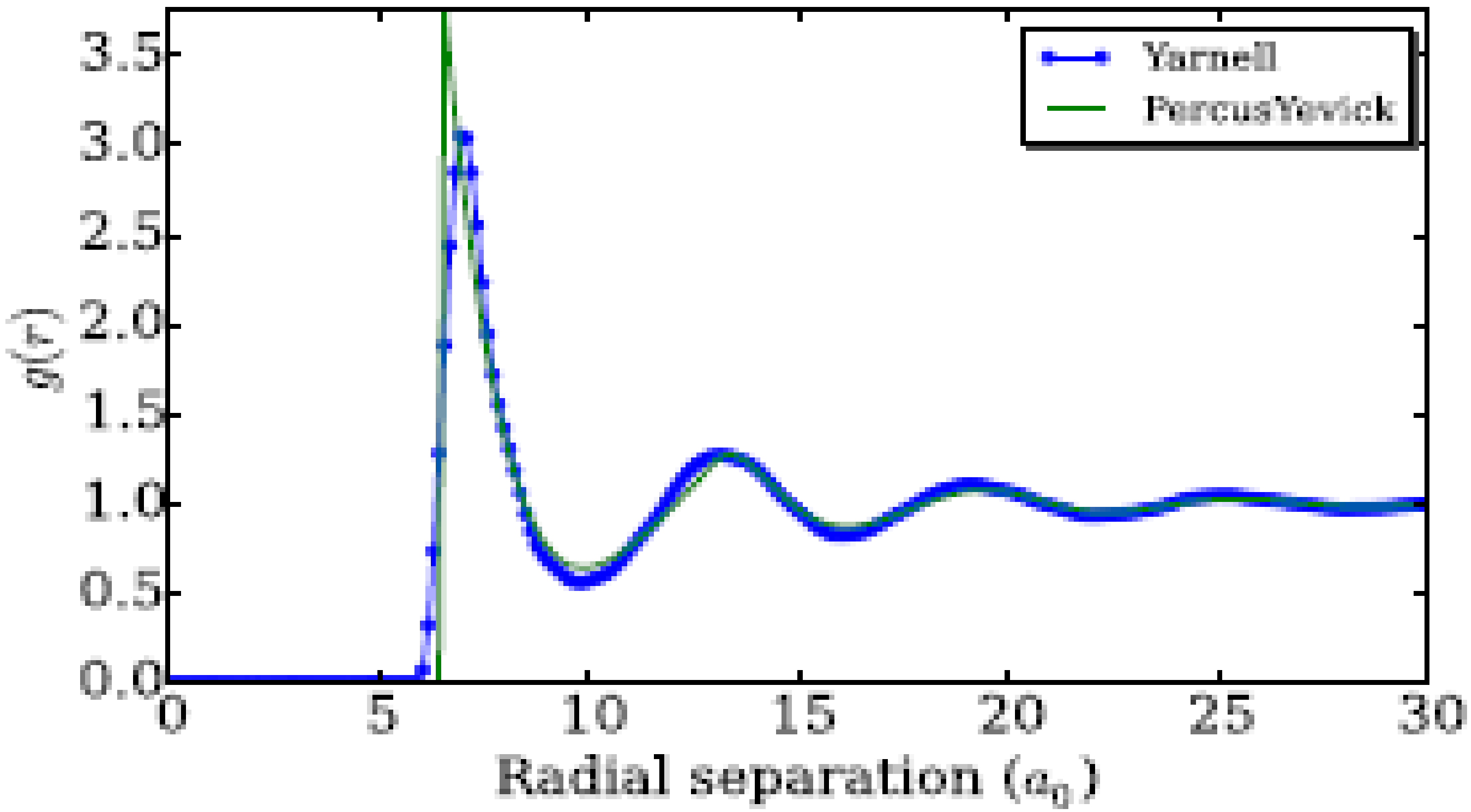

FIG. 2. Pair correlator for argon, as reported in Yarnell,[28] measured in neutron scattering experiments. Also plotted is the pair correlator calculated in the analytical Percus-Yevick approximation as used by Lekner.[9]

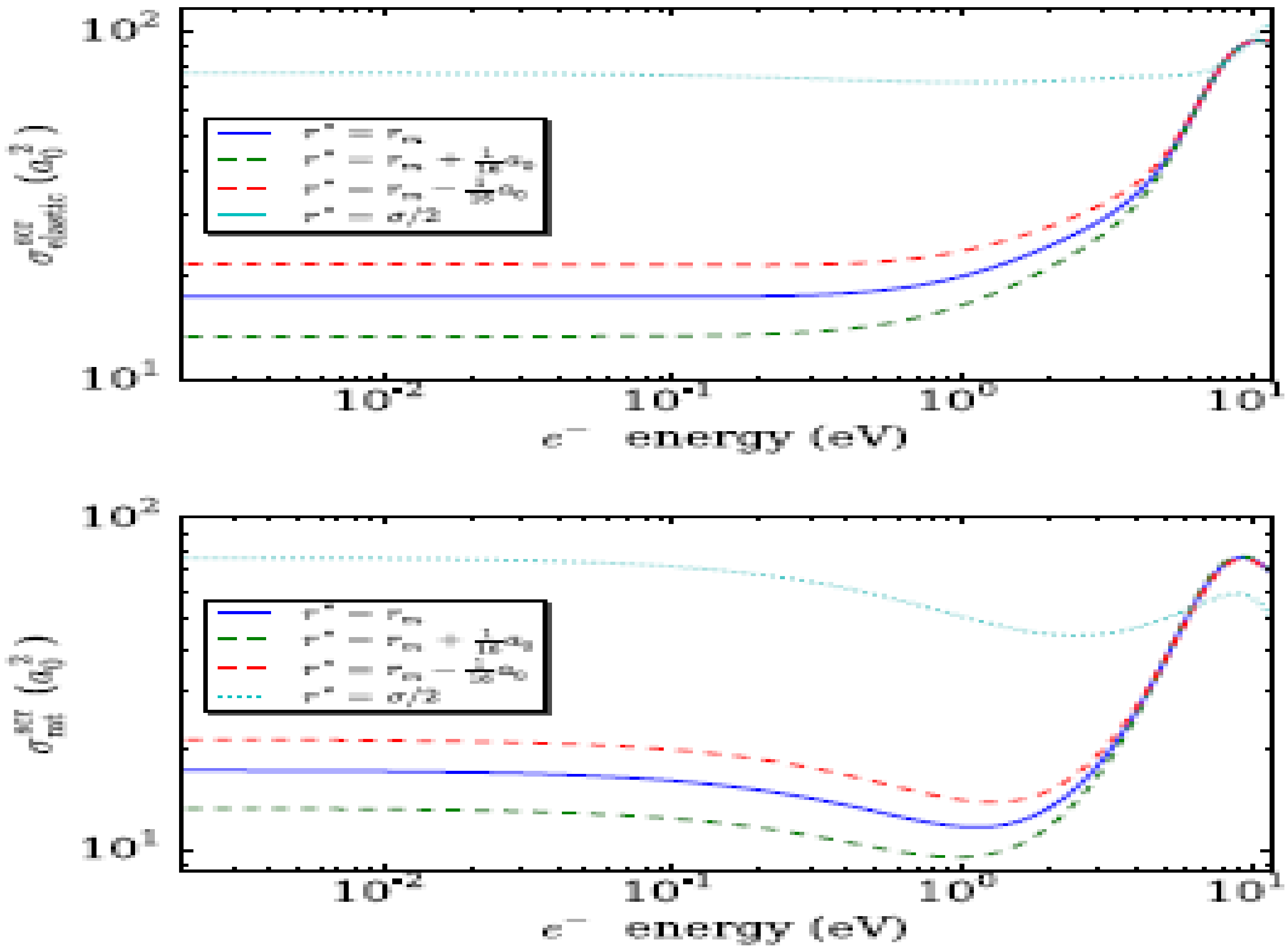

FIG. 5. Screened elastic total and momentum-transfer cross-sections for argon calculated from the phase shifts determined at a distance r^*. Our preferred choice for transport calculations in this paper, $r^* = r_m$, corresponds to the solid line, the dashed lines are those corresponding to a variations $r^* = r_m \pm \frac{1}{18} a_0$, and the dotted line corresponds to a variation of $r^* = \sigma_{\text{core}}/2$.