Bayes Days 2000 at LANL

Three-Day Minicourse on Bayesian Analysis in Physics

Lectures presented by

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Max Planck Institute for Plasma Physics

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For more information, look on the web:
http://public.lanl.gov/kmh/course/BD2000.html

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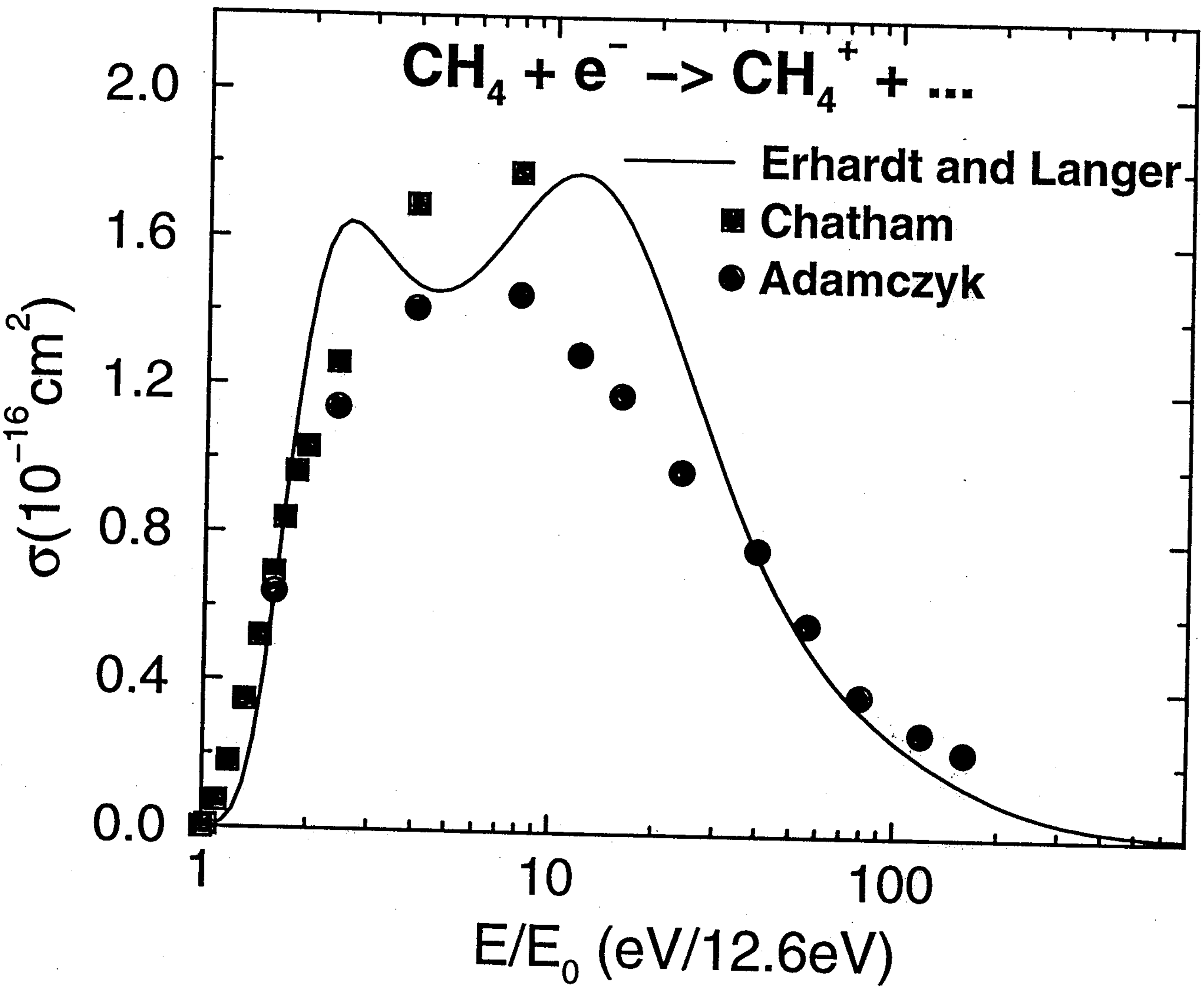
Max-Planck-Institut für Plasmaphysik
Abteilung Oberflächenphysik

Cross sections for partial electron impact ionization of CH_4 and H_2

V. Dose, P. Pecher and R. Preuss

FIGURES



$CH_4 + e^- -> CH_4^+ + ...$
Erhardt and Langer
Chatham
Adamczyk
2.0
1.6
1.2
0.8
0.4
0.0
$\sigma(10^{-16}cm^2)$
1
10
100
E/E_0 (eV/12.6eV)

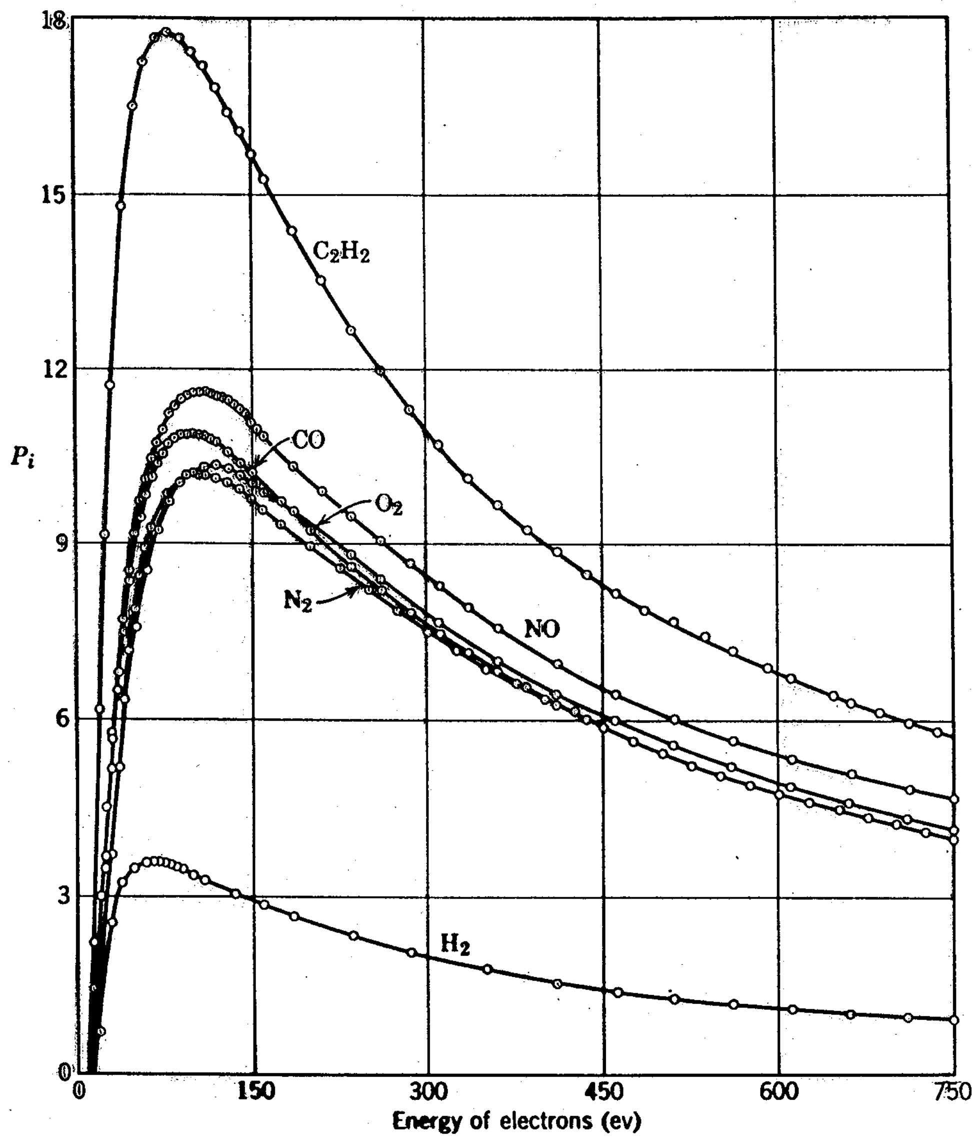
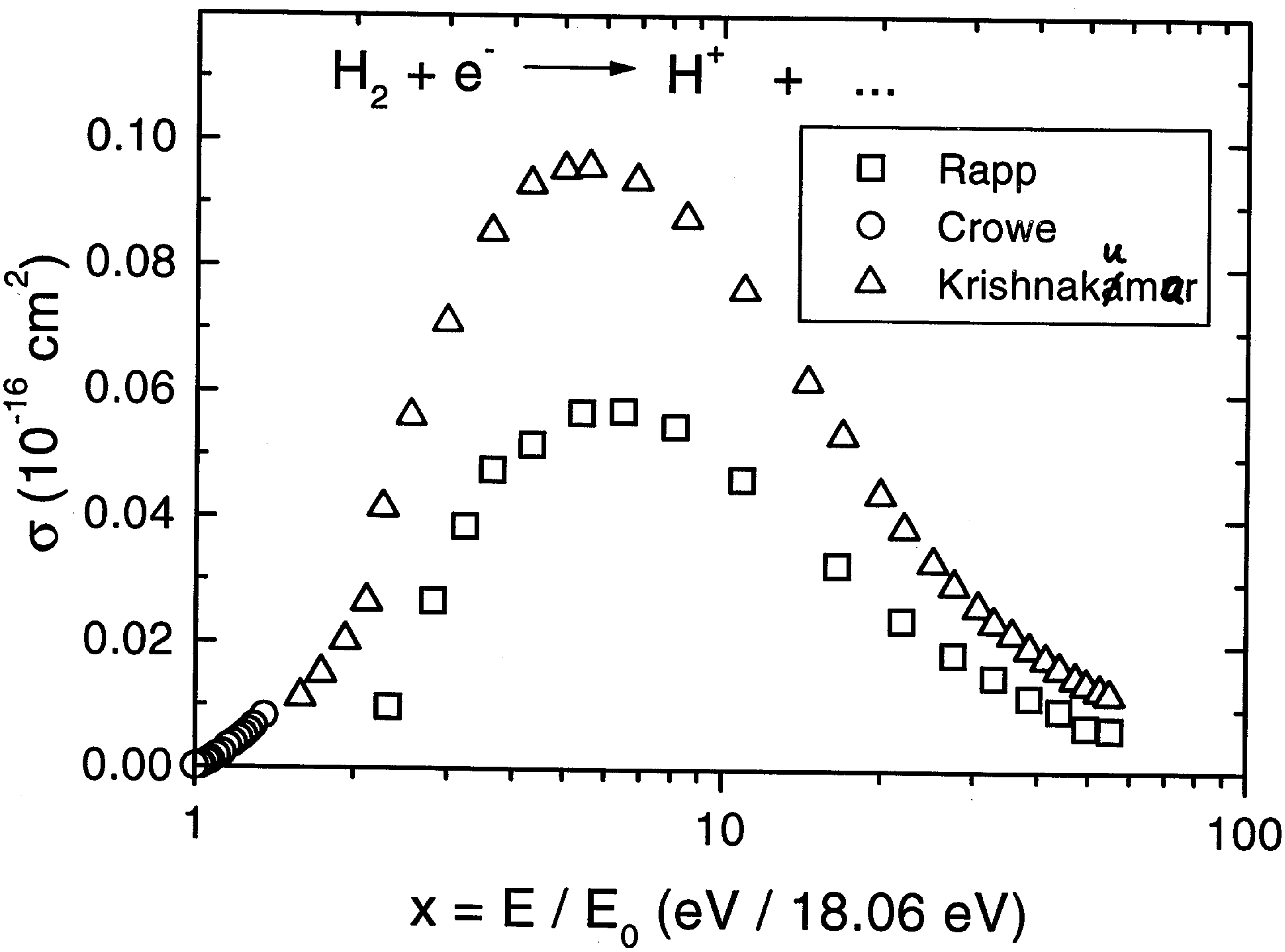


FIG. 5-3-11. The probability of ionization of N_2, CO, O_2, NO, H_2 and C_2H_2. The ordinate represents the number of positive charges per electron per cm path at 1 mm Hg pressure and 0°C. J. T. Tate and P. T. Smith, *Phys. Rev.* **39**, 270 (1932).



unterschiedliche Messbereiche
verschiedene Absolutkalibrierung

The data

1st set: $\vec{\delta}$, $\vec{x}$, $\vec{s}$
2nd set: $\vec{\Delta}$, $\vec{X}$, $\vec{S}$

$$p\left(\vec{\delta}, \vec{\Delta}|\vec{x}, \vec{X}, \vec{s}, \vec{S}, I\right) = p\left(\vec{\delta}|\vec{x}, \not{\vec{X}}, \vec{s}, \not{\vec{S}}, I\right) \cdot p\left(\vec{\Delta}|\not{\vec{\delta}}, \not{\vec{x}}, \vec{X}, \not{\vec{s}}, \vec{S}, I\right)$$

The model

$$\delta_i - c \cdot \varphi\left(x_i, \vec{\lambda}\right) = \alpha_i, \qquad \langle \alpha_i^2 \rangle = s_i^2$$

$$\gamma \Delta_j - \varphi\left(X_i, \vec{\lambda}\right) = \beta_j, \qquad \langle \beta_j^2 \rangle = S_j^2$$

$$p\left(\vec{\delta}|\vec{x}, c, \vec{\lambda}, I\right) = \prod_i \frac{1}{s_i\sqrt{2\pi}} \exp\left\{-\frac{1}{2}\left(\frac{\delta_i - c\varphi_i\left(\vec{\lambda}\right)}{s_i}\right)^2\right\}$$

$$p\left(\vec{\Delta}|\vec{X}, c, \vec{\lambda}, \gamma, I\right) = \prod_j \frac{\gamma}{S_i\sqrt{2\pi}} \exp\left\{-\frac{1}{2}\left(\frac{\gamma\Delta_j - c\varphi_j\left(\vec{\lambda}\right)}{S_j}\right)^2\right\}$$

define:

$$\begin{aligned} \varphi\left(x_i, \vec{\lambda}\right)/s_i &= f_i \qquad & \varphi\left(X_j, \vec{\lambda}\right)/S_j &= F_j \\ \delta_i/s_i &= d_i \qquad & \Delta_j/S_j &= D_j \end{aligned}$$

The likelihood

$$p\left(\vec{d}, \vec{D}|\vec{x}, \vec{X}, c, \vec{\lambda}, \gamma, I\right) =$$
$$(2\pi)^{-n/2} \exp\left\{-\frac{1}{2}\left(\vec{d} - c\vec{f}\right)^T \left(\vec{d} - c\vec{f}\right)\right\} \cdot$$
$$(2\pi)^{-N/2}\gamma^N \exp\left\{-\frac{1}{2}\left(\gamma\vec{D} - c\vec{F}\right)^T \left(\gamma\vec{D} - c\vec{F}\right)\right\}$$

model functions (Born-Bethe)

1. $\sigma(E) \sim \ln x/x, \qquad x = E/E_0 \geq 1$

$$\varphi(E) = \frac{(x-1)^\epsilon \ln x}{a + (x-1)^\epsilon \cdot x}, \qquad \sigma(E) = c \cdot \varphi(E)$$

2. $\sigma(E) \sim 1/x$

$$\varphi(E) = \frac{(x-1)^\epsilon}{a + (x-1)^\epsilon \cdot x}, \qquad \sigma(E) = c \cdot \varphi(E)$$

Which model applies ? What are the numerical values of c and $\vec{\lambda}$?

Bayes' Theorem

$$p\left(c, \vec{\lambda}, \gamma | \vec{d}, \vec{x}, \vec{D}, \vec{X}, I\right) = \frac{p\left(c, \gamma, \vec{\lambda} | I\right)}{p\left(\vec{d}, \vec{D} | \vec{x}, \vec{X}, I\right)} \cdot p\left(\vec{d}, \vec{D} | \vec{x}, \vec{X}, c, \gamma, \vec{\lambda}, I\right)$$

$$p\left(\vec{d}, \vec{D} | \vec{x}, \vec{X}, I\right) = \int p\left(\vec{d}, \vec{D}, c, \gamma, \vec{\lambda} | \vec{x}, \vec{X}, I\right) \mathrm{d}c\mathrm{d}\gamma\mathrm{d}\vec{\lambda} = \int p\left(c, \gamma, \vec{\lambda} | I\right) \cdot p\left(\vec{d}, \vec{D} | \vec{x}, \vec{X}, c, \gamma, \vec{\lambda}, I\right) \mathrm{d}c\mathrm{d}\gamma\mathrm{d}\vec{\lambda}$$

Priors $\left(\vec{\lambda} = (a, \epsilon)\right)$

$$p\left(c, \gamma, \vec{\lambda} | I\right) = p(c|I)p(\gamma|I)p(a|I)p(\epsilon|I)$$

1. $c > 0, \qquad p(c|I) = 1/c_{\mathrm{max}}$

2. $g = \langle\gamma\rangle, \qquad p(\gamma|I) = \exp\{-\gamma/g\}/g$

3. $a > 0, \qquad p(a|I) = 1/a_{\mathrm{max}}$

4. $\epsilon > 0, \qquad p(\epsilon|I) = \frac{1}{2\sqrt{2\pi}} \exp\left\{-\frac{1}{2}\left(\frac{\epsilon}{2}\right)^2\right\}$

The problem with the global likelihood

$$p(H|D,I) = \frac{p(H|I)}{p(D|I)} \cdot p(D|H,I)$$

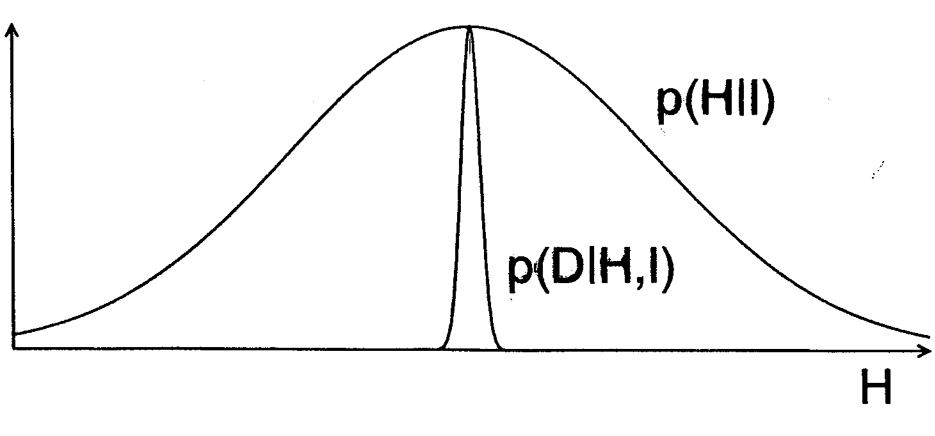
$$\int p(H|I)\ dH = 1\ , \quad \int p(D|H,I)\ d^E D = 1$$

but

$$\int p(D|H,I)\ dH = \text{unknown}$$

and may not even be finite.

$$p(D|I)\ dH = \int \underbrace{p(H|I)}_{\text{sampling density}} \quad p(D|H,I)\ dH$$



Parameters

$$\langle \xi^n \rangle = \int \xi^n \left\{ \frac{p\left(c,\gamma,a,\epsilon|I\right) p\left(\vec{d},\vec{D}|\vec{x},\vec{X},c,a,\gamma,\epsilon,I\right)}{p\left(\vec{d},\vec{D}|\vec{x},\vec{X},I\right)} \right\} \mathrm{d}c\mathrm{d}\gamma\mathrm{d}a\mathrm{d}\epsilon$$

Covariances

$$C_{ik} = \langle \xi_i \xi_k \rangle - \langle \xi_i \rangle \langle \xi_k \rangle$$

$$G(\xi,\mathrm{C}^{-1}) = G_0 \exp\left\{ -\frac{1}{2} \left(\vec{\xi} - \langle\vec{\xi}\rangle\right)^T \mathrm{C}^{-1} \left(\vec{\xi} - \langle\vec{\xi}\rangle\right) \right\}$$

Global likelihood

$$p\left(\vec{d},\vec{D}|\vec{x},\vec{X},I\right) = \int p\left(c,\gamma,a,\epsilon|I\right) p\left(\vec{d},\vec{D}|\vec{x},\vec{X},c,a,\gamma,\epsilon,I\right) \mathrm{d}c\mathrm{d}\gamma\mathrm{d}a\mathrm{d}\epsilon = \int \underbrace{G^*\left(\vec{\xi},\mathrm{C}^{-1}\right)} \underbrace{\left\{ \frac{p\left(c,\gamma,a,\epsilon|I\right) p\left(\vec{d},\vec{D}|\vec{x},\vec{X},c,\gamma,a,\epsilon,I\right)}{G^*\left(\vec{\xi},\mathrm{C}^{-1}\right)} \right\}} \mathrm{d}c\mathrm{d}\gamma\mathrm{d}a\mathrm{d}\epsilon$$

Sampling density "integrand" slowly varying

Channel	M(25a)/M(25b)	c	a	ε	E_0/eV
$CH_4 + e^- \rightarrow CH_4^+ + \ldots$	$2 \cdot 10^3 : 1$	9.7	4.4	0.14	12.6
$CH_4 + e^- \rightarrow CH_3^+ + \ldots$	$10^3 : 1$	6.7	3.5	0.20	14.3
$CH_4 + e^- \rightarrow CH_2^+ + \ldots$	$10^4 : 1$	0.93	4.0	1.0	15.1
$CH_4 + e^- \rightarrow CH^+ + \ldots$	$26 : 1$	0.31	0.67	1.7	22.2
$CH_4 + e^- \rightarrow C^+ + \ldots$	$1 : 2 \cdot 10^2$	0.22	8.7	1.2	25.0
$CH_4 + e^- \rightarrow H^+ + \ldots$	[redacted]	1.3	22	1.2	18.1
$H_2 + e^- \rightarrow H_2^+ + \ldots$	$10^{10} : 1$	3.9	1.8	0.18	15.43
$H_2 + e^- \rightarrow H^+ + \ldots$	[redacted]	0.91	34	1.5	18.06

TABLE I. Posterior estimates for the model parameters in Eqn. (25a,b).

Posterior cross sections

$$\langle \sigma^k(z) \rangle = \int \sigma^k p\left(\sigma | z, \vec{d}, \vec{D}, \vec{x}, \vec{X}, I\right) \mathrm{d}\sigma$$

$$p\left(\sigma | z, \vec{d}, \vec{D}, \vec{x}, \vec{X}, I\right) =$$
$$\int p\left(\sigma, c, \gamma, a, \epsilon | z, \vec{d}, \vec{D}, \vec{x}, \vec{X}, I\right) \mathrm{d}c\mathrm{d}\gamma\mathrm{d}a\mathrm{d}\epsilon =$$
$$\int p\left(c, \gamma, a, \epsilon | \not{z}, \vec{d}, \vec{D}, \vec{x}, \vec{X}, I\right) \cdot p\left(\sigma | z, c, \gamma, a, \epsilon, \vec{d}, \vec{D}, \vec{x}, \vec{X}, I\right) \mathrm{d}c\mathrm{d}\gamma\mathrm{d}a\mathrm{d}\epsilon$$

$$p\left(c, \gamma, a, \epsilon | \vec{d}, \vec{D}, \vec{x}, \vec{X}, I\right) = \frac{p\left(c, \gamma, a, \epsilon | I\right) p\left(\vec{d}, \vec{D} | \vec{x}, \vec{X}, c, \gamma, a, \epsilon, I\right)}{p\left(\vec{d}, \vec{D} | \vec{x}, \vec{X}, I\right)}$$

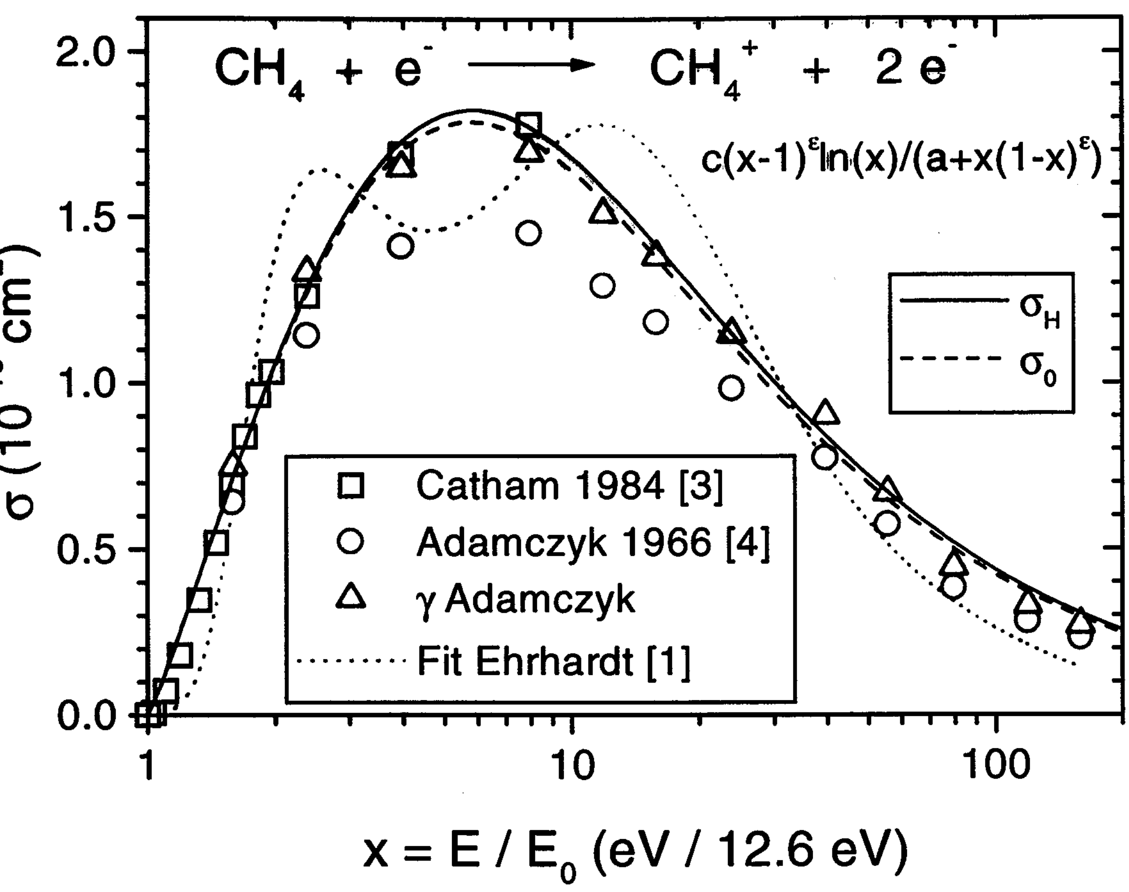
sampling density as for parameter estimation

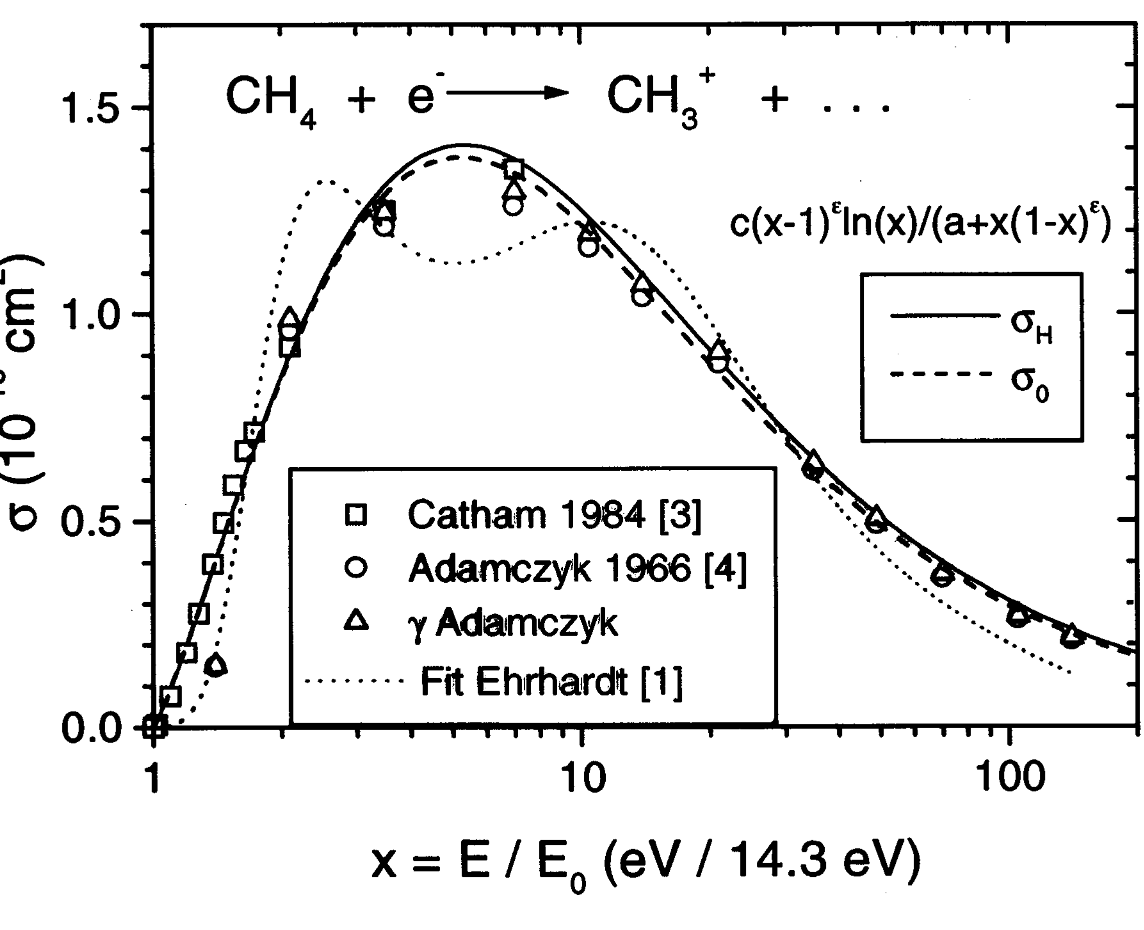
$$p\left(\sigma | z, c, \not{\gamma}, a, \epsilon, \not{\vec{d}}, \not{\vec{D}}, \not{\vec{x}}, \not{\vec{X}}, I\right) = p\left(\sigma | z, c, a, \epsilon\right)$$

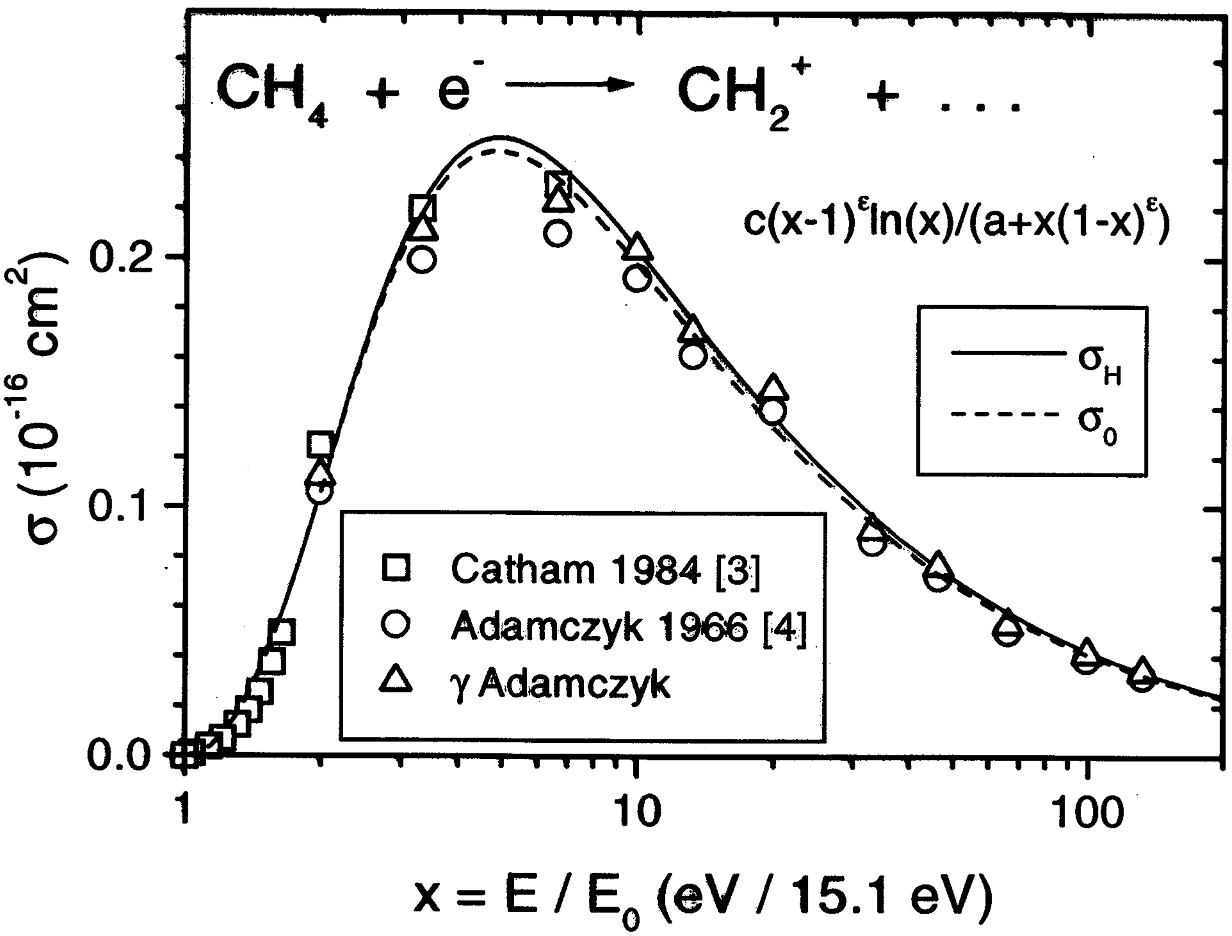
$$p\left(\sigma | z, c, \not{\gamma}, a, \epsilon\right) = \delta\left(\sigma - c\varphi(z, a, \epsilon)\right)$$

$$\langle \sigma^k(z) \rangle = \int \left\{c\varphi(z, a, \epsilon)\right\}^k p\left(c, \gamma, a, \epsilon | \vec{d}, \vec{D}, \vec{x}, \vec{X}, I\right) \mathrm{d}x\mathrm{d}\gamma\mathrm{d}a\mathrm{d}\epsilon$$

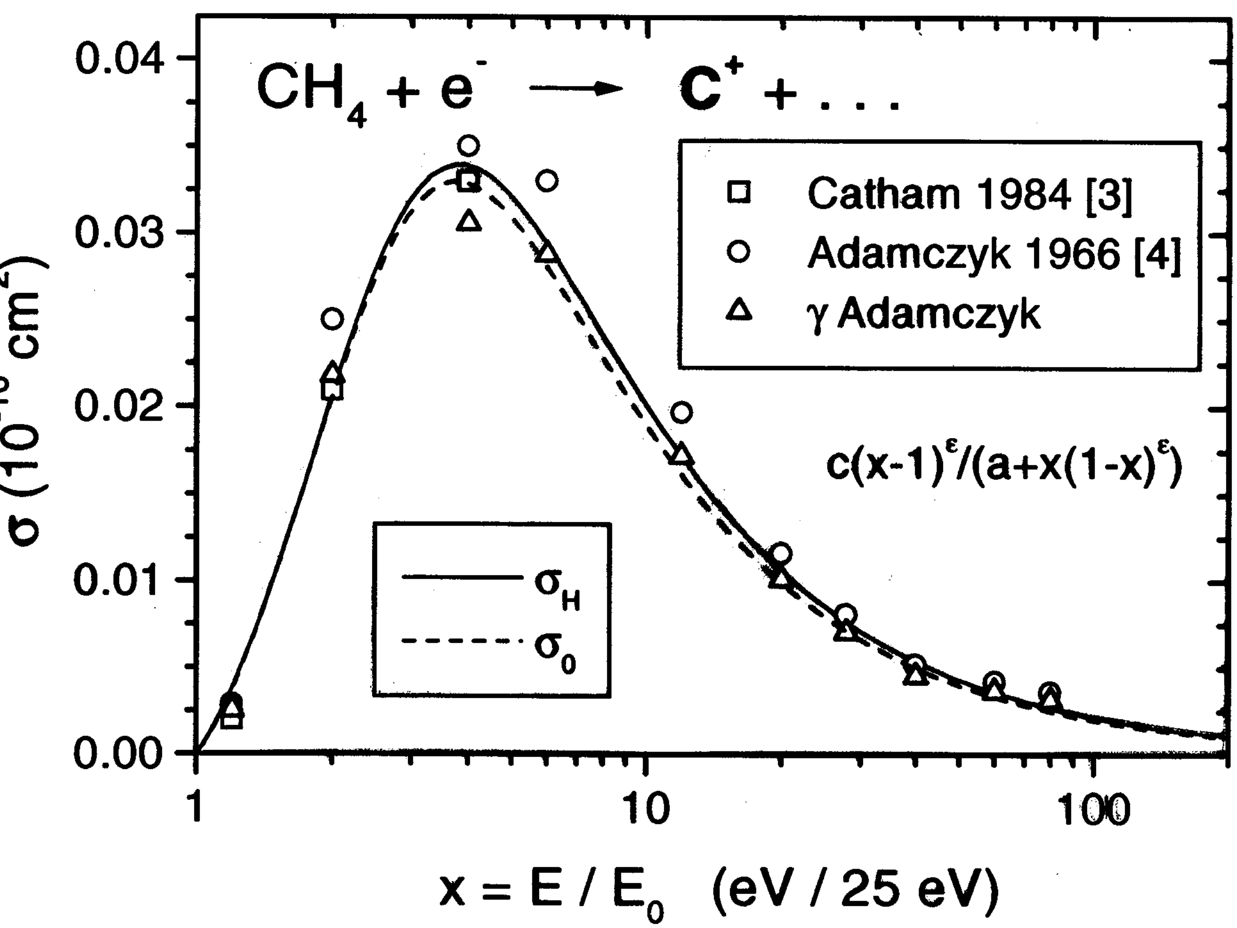
$$\langle \sigma(z) \rangle, \langle \Delta\sigma^2(z) \rangle$$


CH4 + e- → CH4+ + 2 e-
c(x-1)^ε ln(x)/(a+x(1-x)^ε)
σH
σ0
Catham 1984 [3]
Adamczyk 1966 [4]
γ Adamczyk
Fit Ehrhardt [1]
σ (10^-16 cm^2)
x = E / E0 (eV / 12.6 eV)

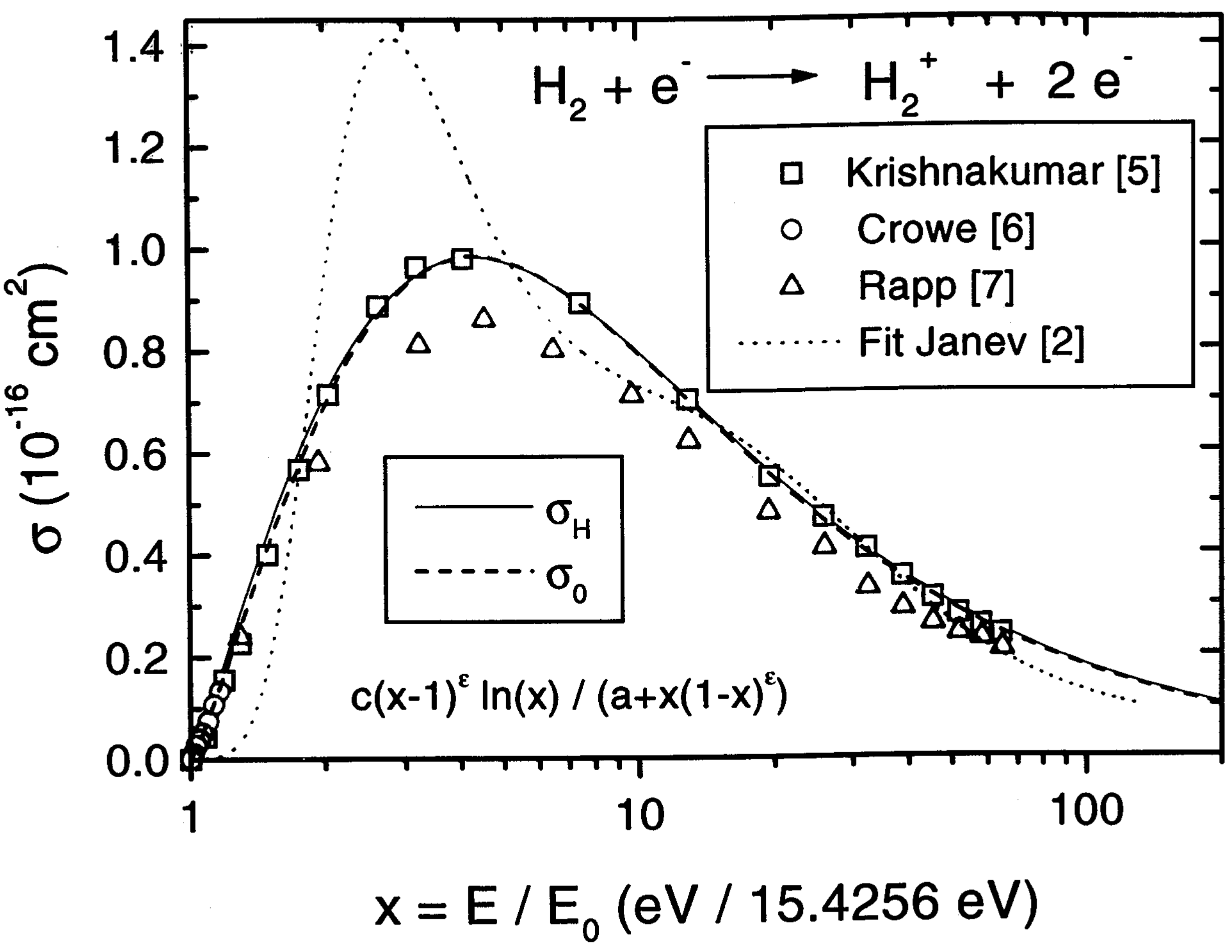

CH4 + e- → CH3+ + . . .
c(x-1)^ε ln(x)/(a+x(1-x)^ε)
σH
σ0
Catham 1984 [3]
Adamczyk 1966 [4]
γ Adamczyk
Fit Ehrhardt [1]
σ (10^-16 cm^2)
x = E / E0 (eV / 14.3 eV)



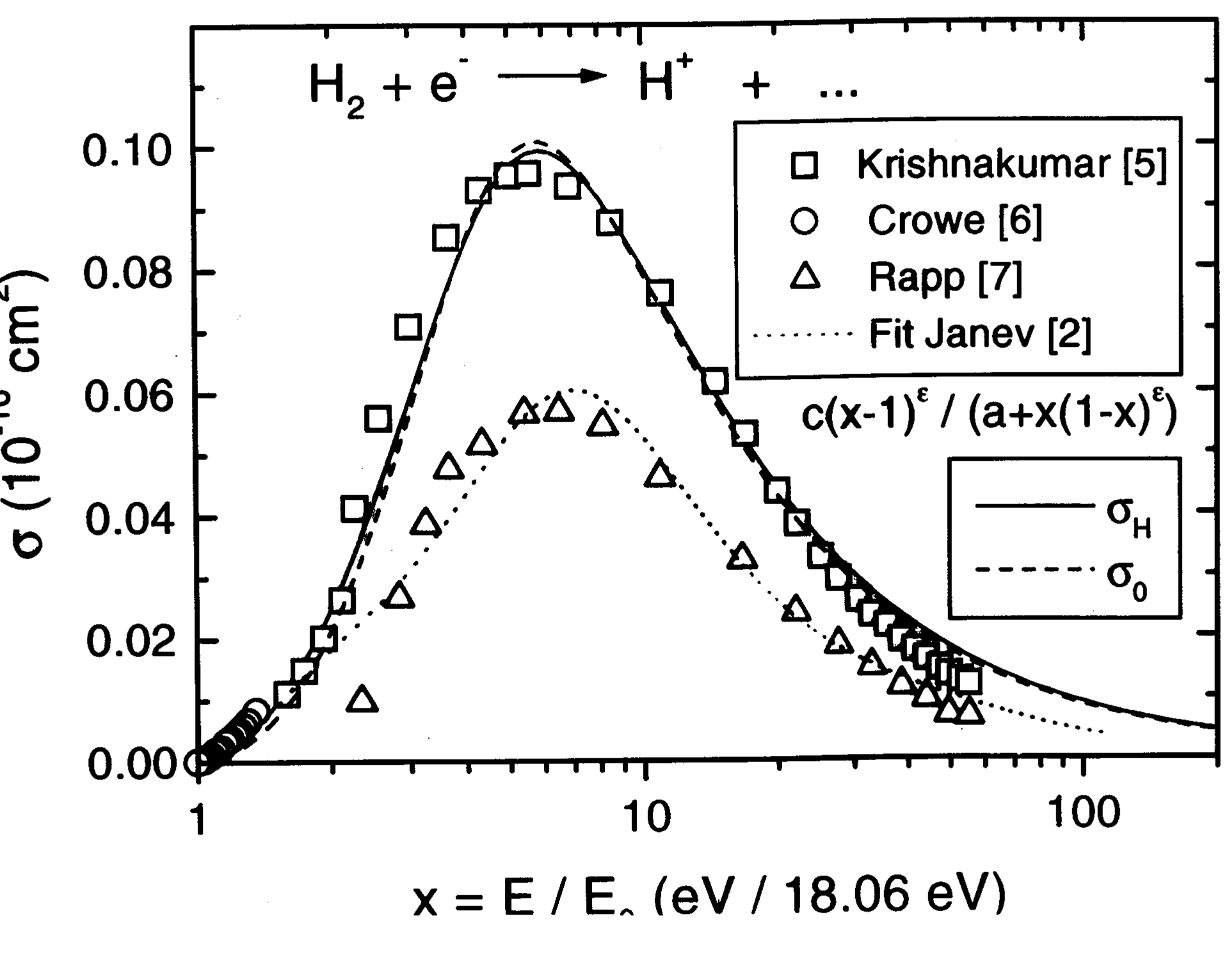
$CH_4 + e^- \rightarrow CH_2^+ + \ldots$
$c(x-1)^\varepsilon \ln(x)/(a+x(1-x)^\varepsilon)$
σ_H
σ_0
Catham 1984 [3]
Adamczyk 1966 [4]
γ Adamczyk
σ (10^{-16} cm^2)
0.0
0.1
0.2
1
10
100
x = E / E_0 (eV / 15.1 eV)



$CH_4 + e^- \rightarrow C^+ + \ldots$
Catham 1984 [3]
Adamczyk 1966 [4]
γ Adamczyk
$c(x-1)^\varepsilon/(a+x(1-x)^\varepsilon)$
σ_H
σ_0
σ (10^{-16} cm^2)
0.00
0.01
0.02
0.03
0.04
1
10
100
x = E / E_0 (eV / 25 eV)



$H_2 + e^- \longrightarrow H_2^+ + 2e^-$
Krishnakumar [5]
Crowe [6]
Rapp [7]
Fit Janev [2]
σ_H
σ_0
$c(x-1)^\varepsilon \ln(x) / (a+x(1-x)^\varepsilon)$
σ (10^{-16} cm^2)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1
10
100
$x = E / E_0$ (eV / 15.4256 eV)



$H_2 + e^- \longrightarrow H^+ + ...$
Krishnakumar [5]
Crowe [6]
Rapp [7]
Fit Janev [2]
$c(x-1)^\varepsilon / (a+x(1-x)^\varepsilon)$
σ_H
σ_0
σ (10^{-16} cm^2)
0.00
0.02
0.04
0.06
0.08
0.10
1
10
100