Elastic and inelastic electron scattering by biomolecules –
the first step towards understanding of basic interactions

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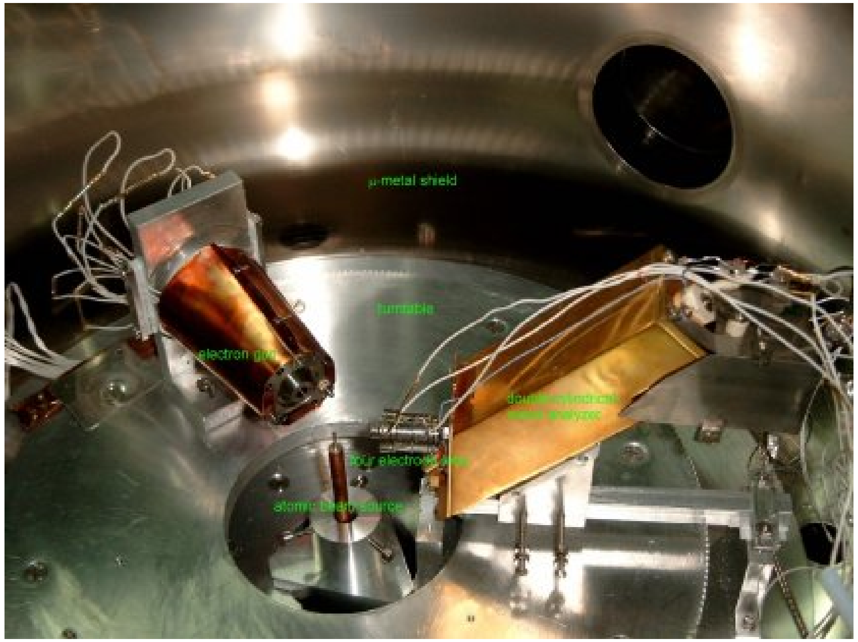
COST WG1 meeting, Lisbon, 23-26.02.2006

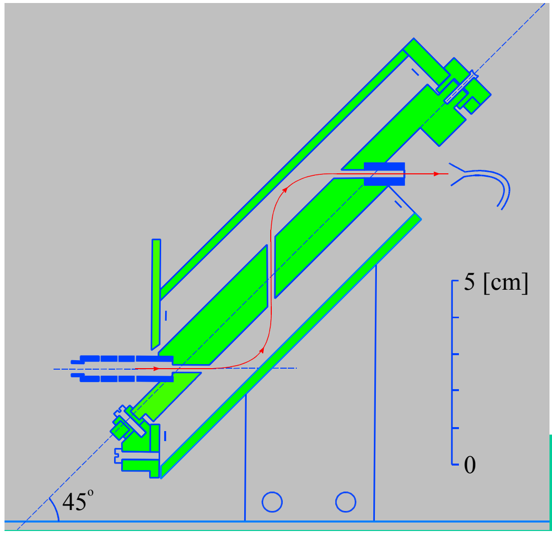
Questions:

- *Why is it the first step towards understanding of basic interactions?*
- *What we can learn from differential cross sections?*
- *What is the relevance of data taken in binary collisions?*

Electron spectrometers:

UGRA – designed for gaseous targets; ESMA – for powders





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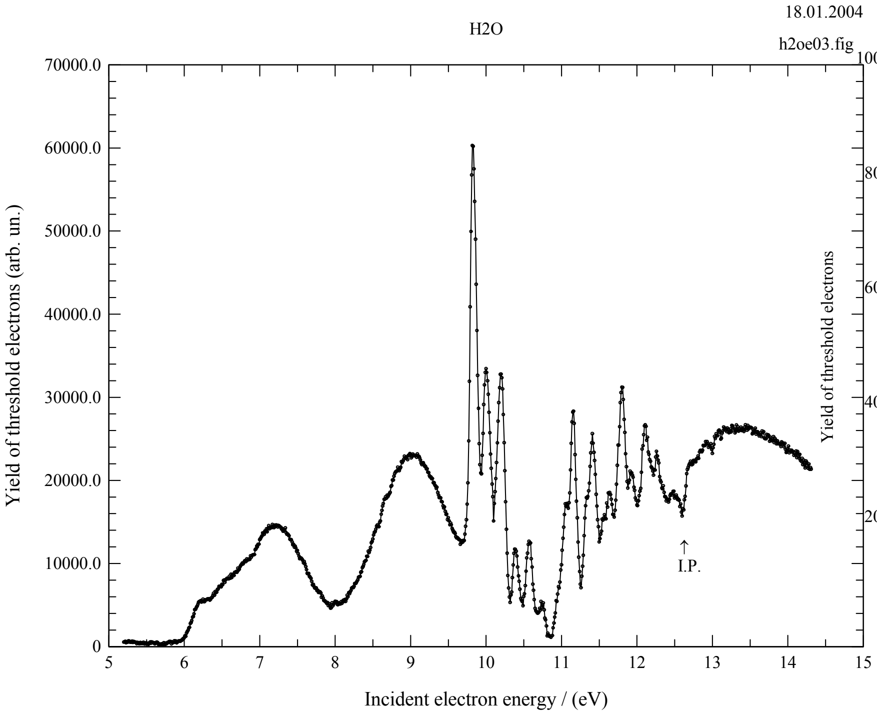
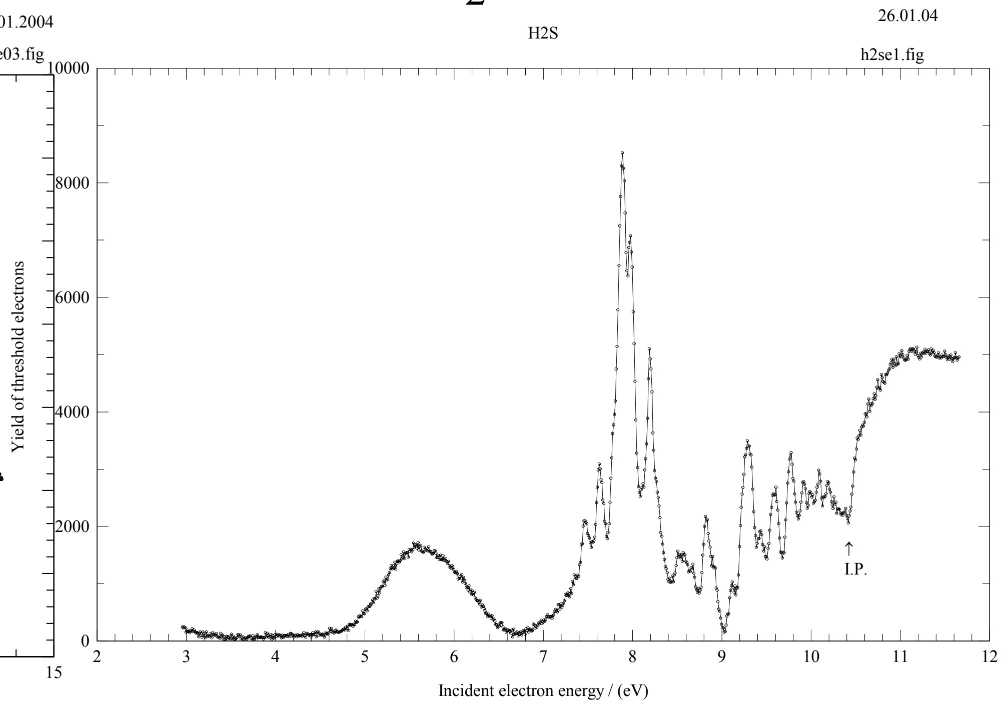
The threshold electron impact spectrum of H_2O

J. Jureta, *Eur. Phys. J. D* **32** (2005) 319

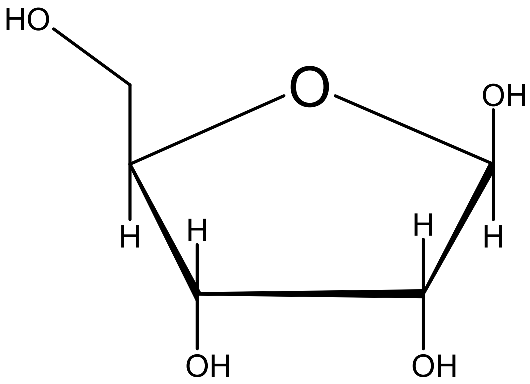
H_2O



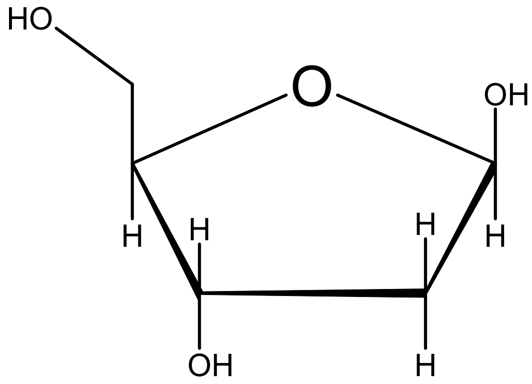
H_2S



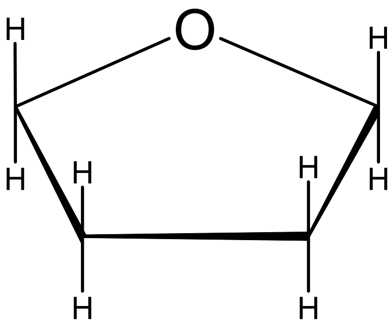
Deoxyribose analogues



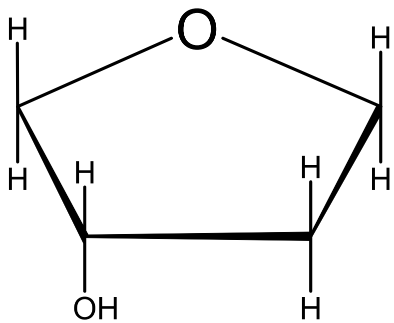
Ribose



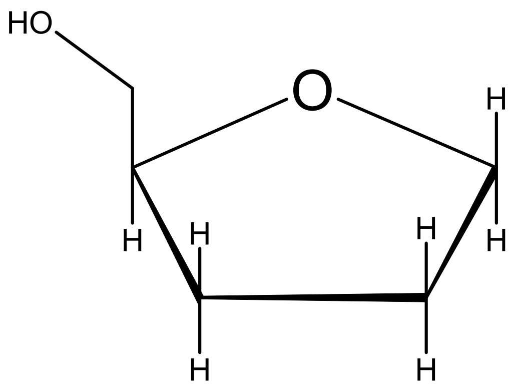
2-deoxy-D-ribose



Tetrahydrofuran
(C_4H_8O)



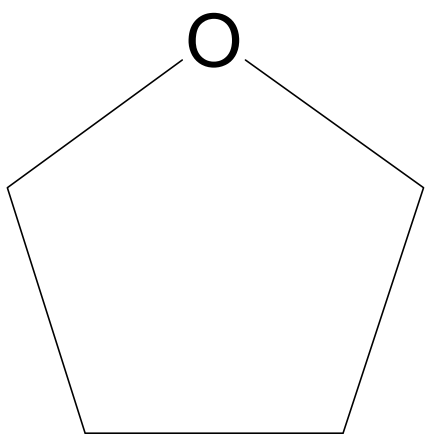
3-hydroxytetrahydrofuran
($C_4H_8O_2$)



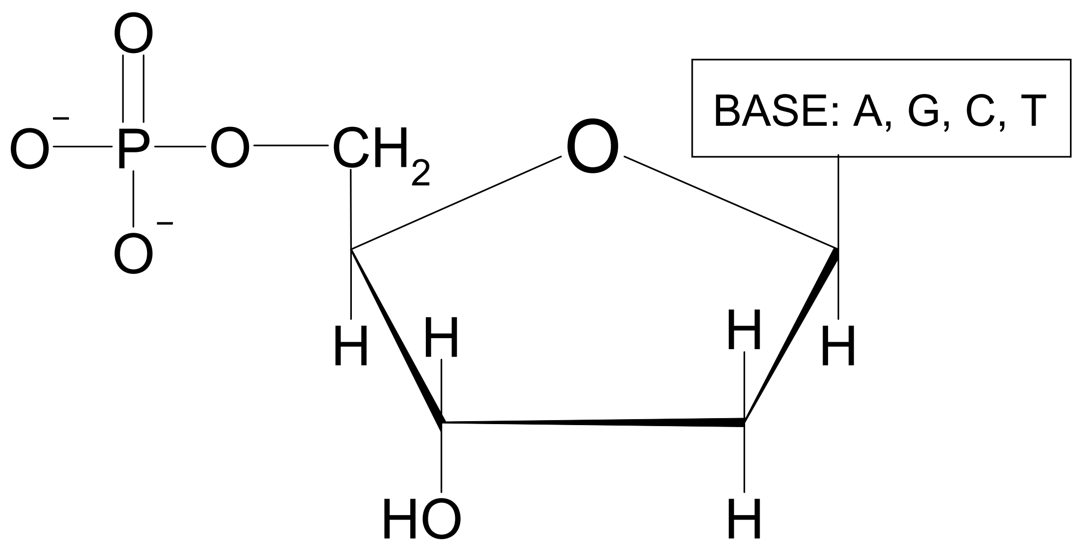
α-tetrahydrofurfuryl alcohol
($C_5H_{10}O_2$)

Electron interactions with THF (tetrahydrofuran) molecule

Energy loss spectra and elastic differential cross sections



THF molecule C_4H_8O



Deoxyribose Analogues

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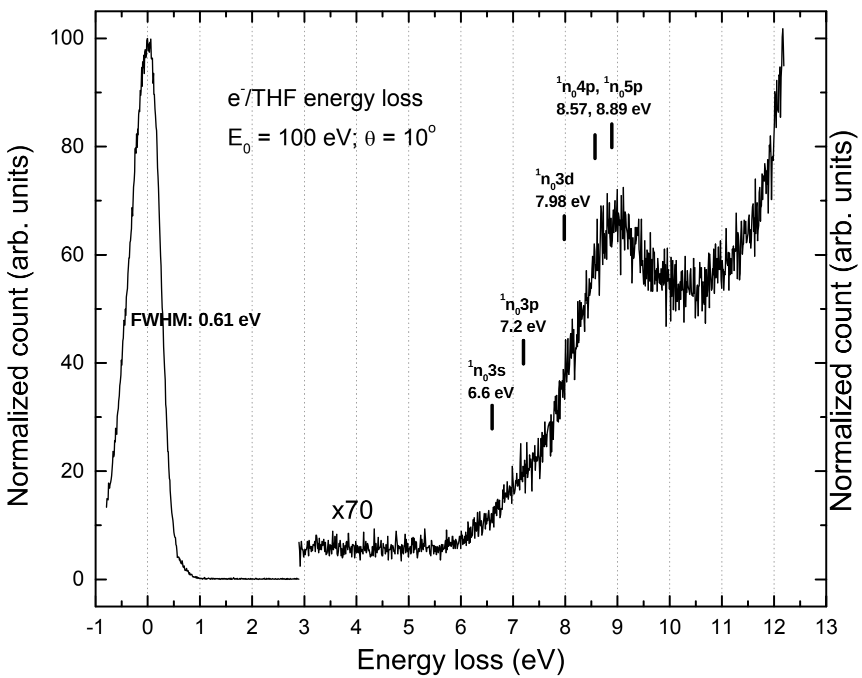
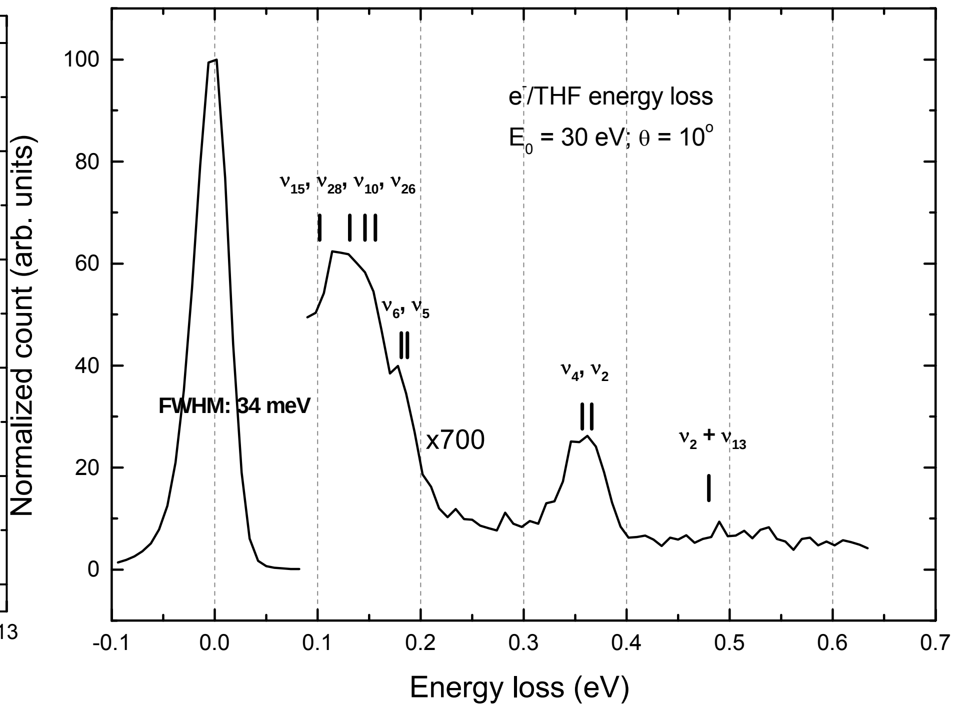
Electron interactions with THF (tetrahydrofuran) molecule

Energy loss spectra and elastic differential cross sections

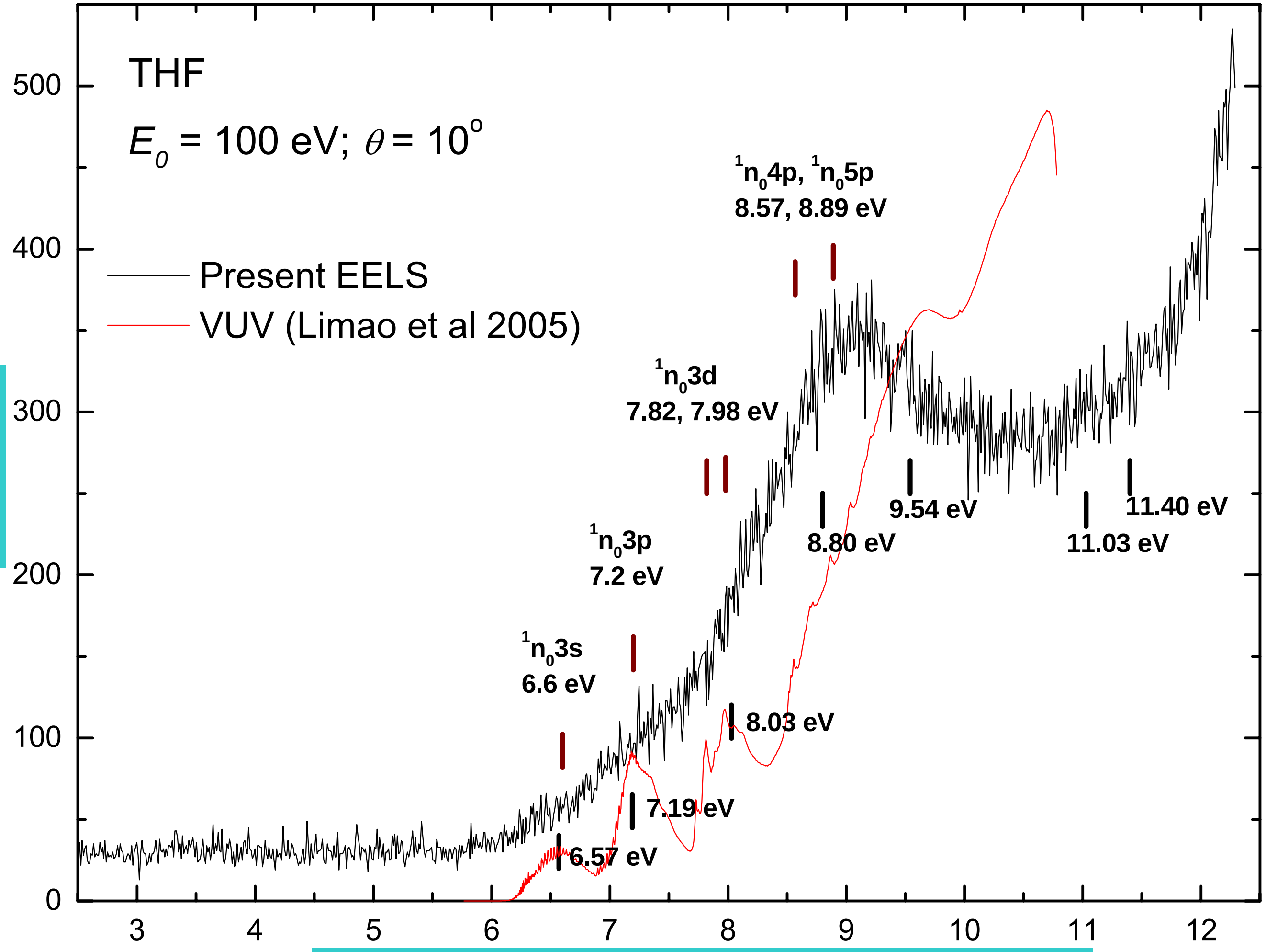




Institute of Physics, Belgrade and University of Liège

Electron interactions with THF (tetrahydrofuran) molecule

Energy loss spectra and elastic differential cross sections



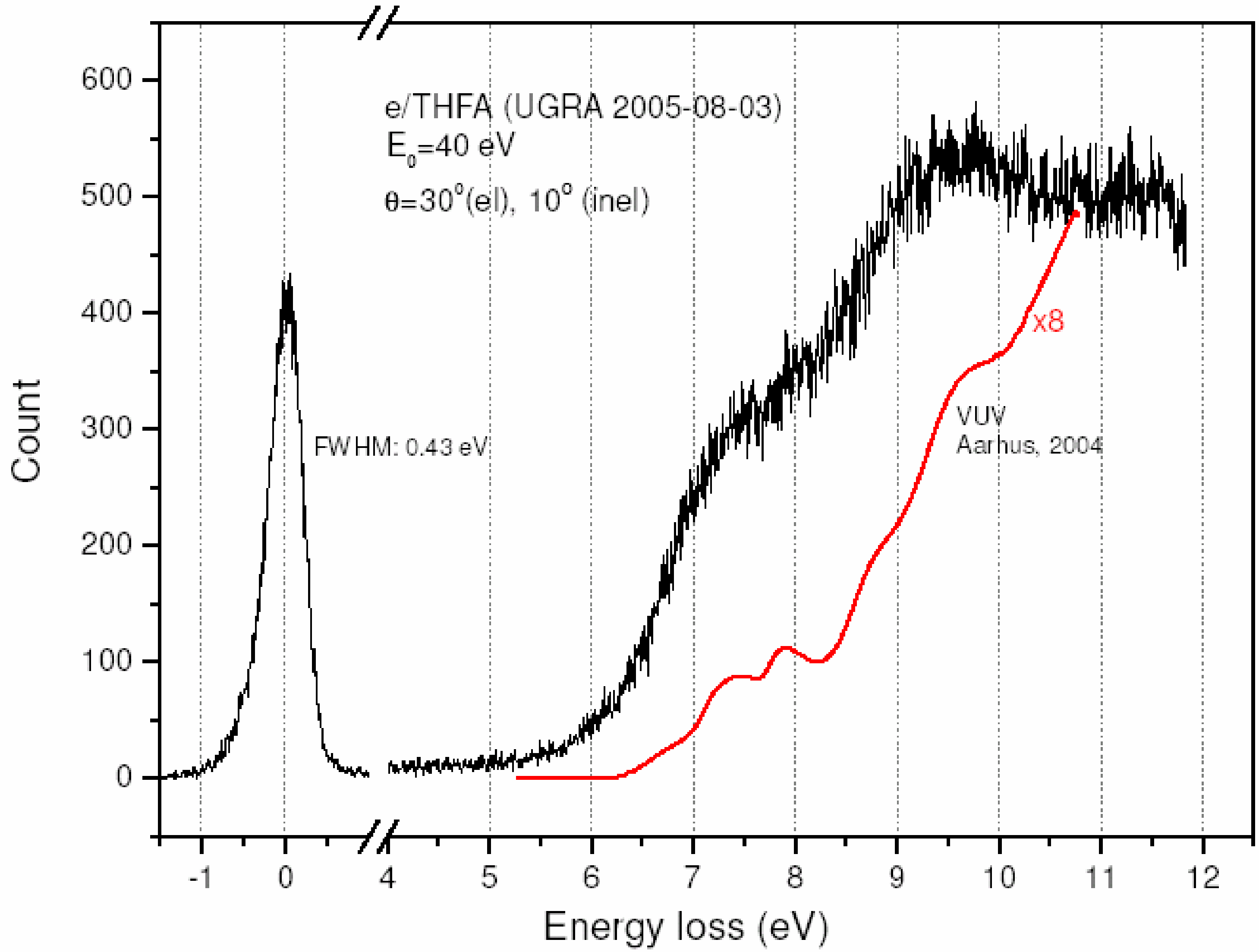
CS (arb.u.)

Electron energy loss (eV)

Institute of Physics, Belgrade; University of Lisbon

Electron interactions with THFA (tetrahydrofuran) molecule

Energy loss spectra and VUV photoabsorption spectra



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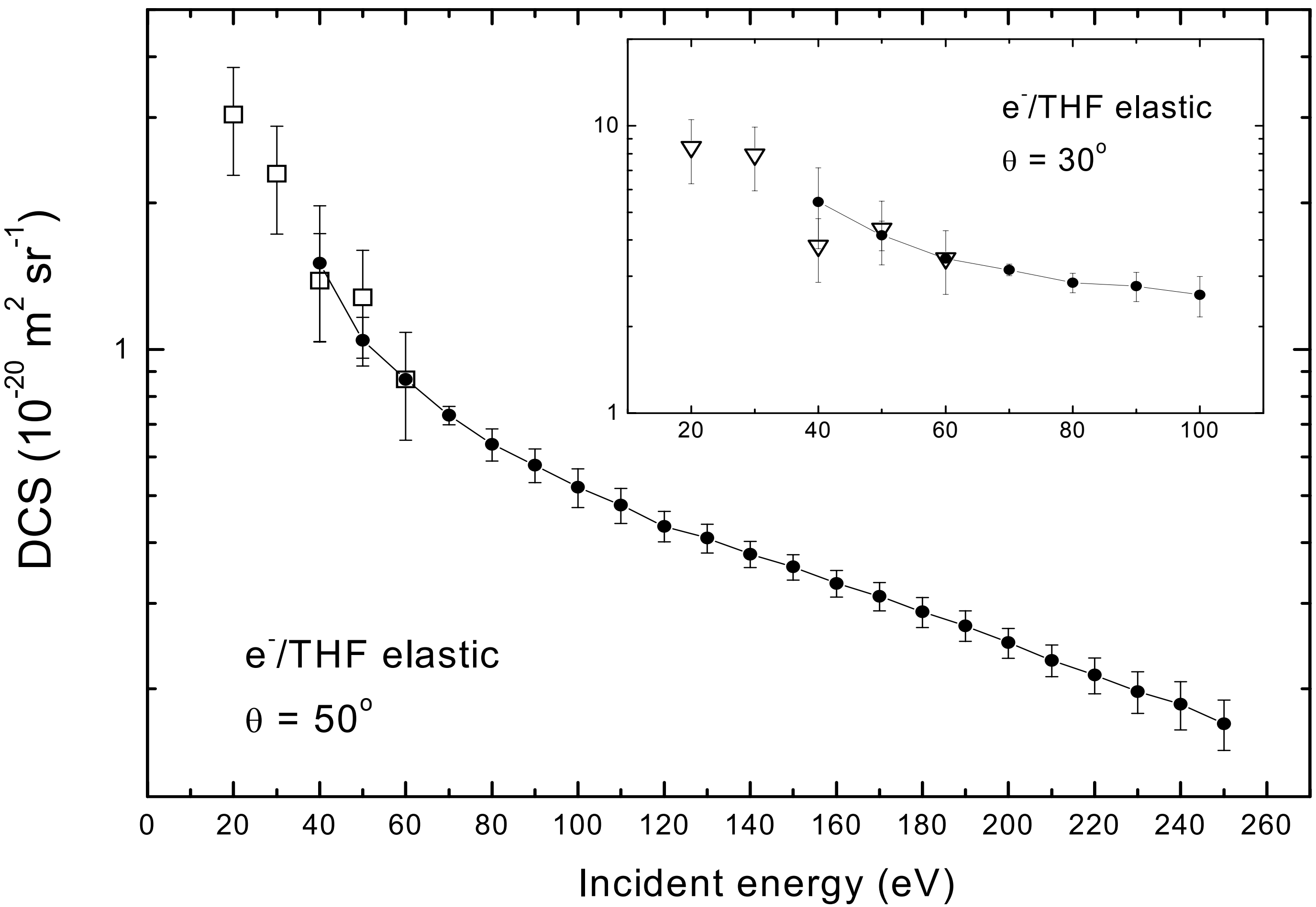
Electron interactions with THF (tetrahydrofuran) molecule

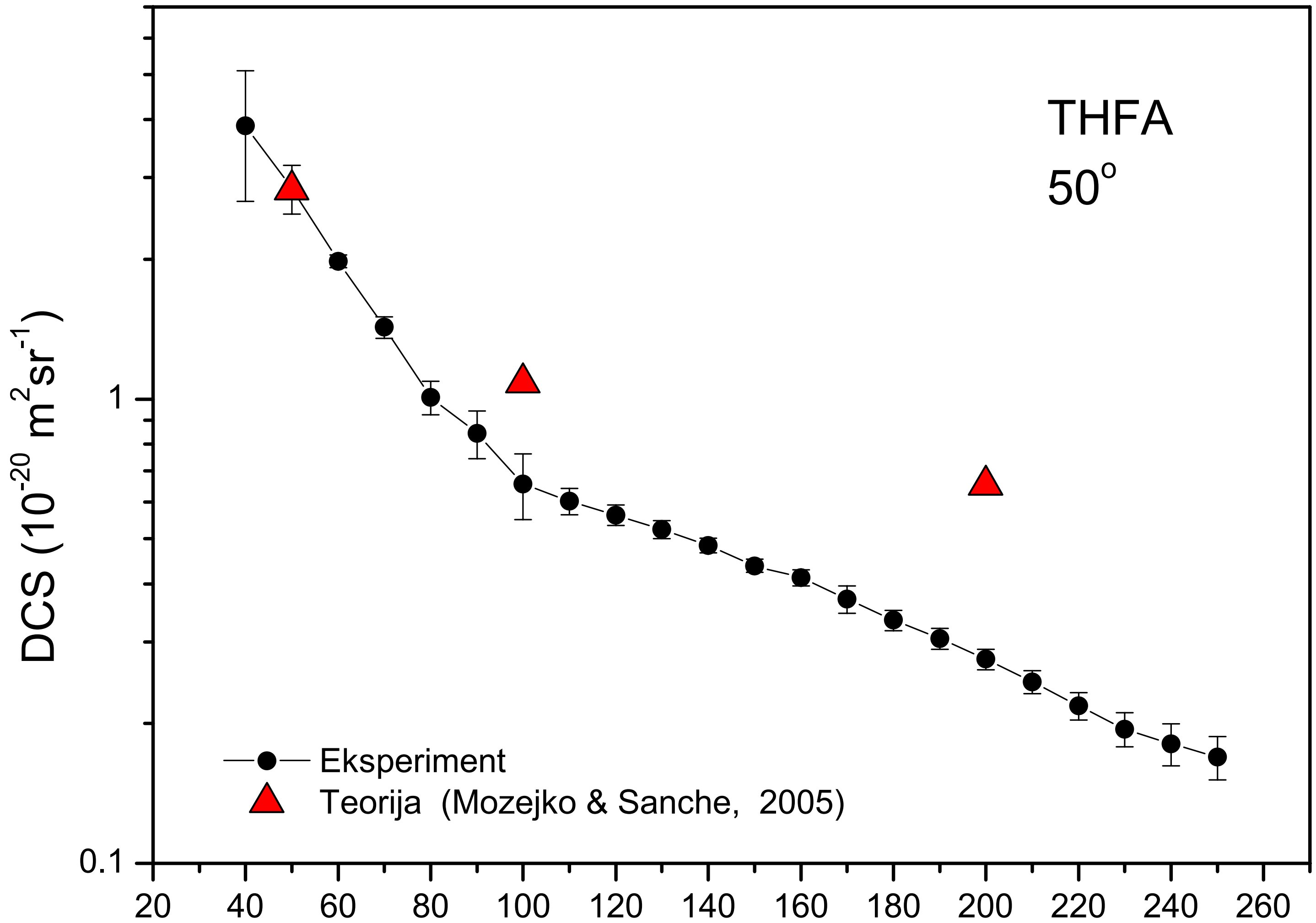
Elastic electron scattering



□,Δ,University of Liège and ●,Institute of Physics, Belgrade

Electron interactions with THFA (tetrahydrofurfuryl alcohol) molecule

Elastic electron scattering



Electron impact energy (eV)

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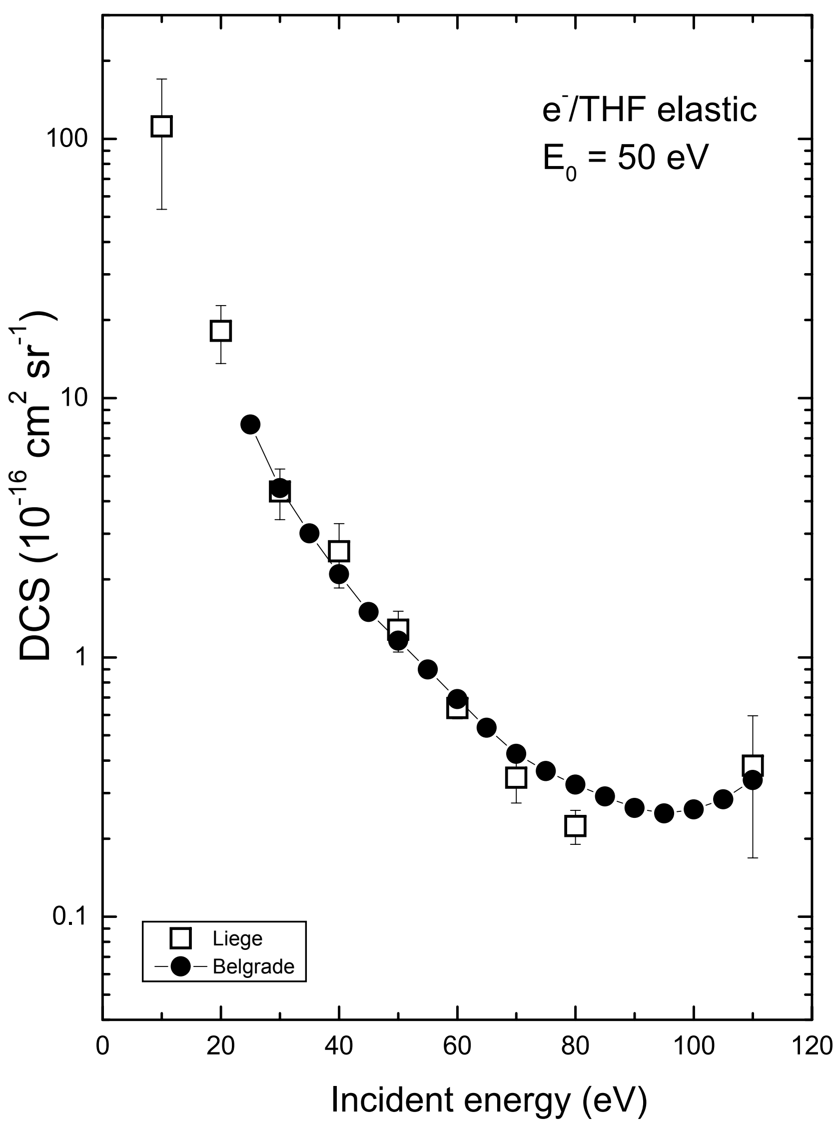
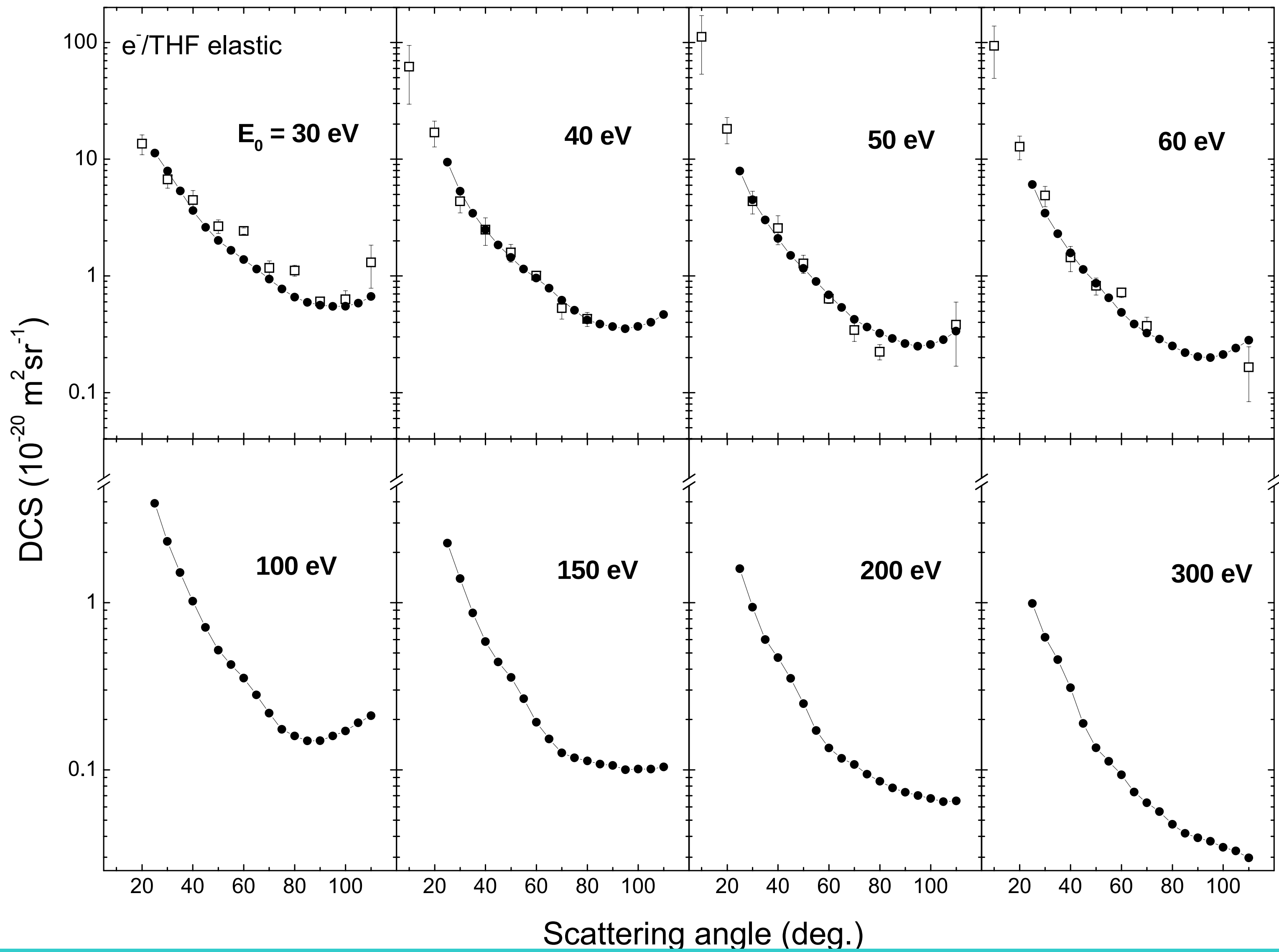


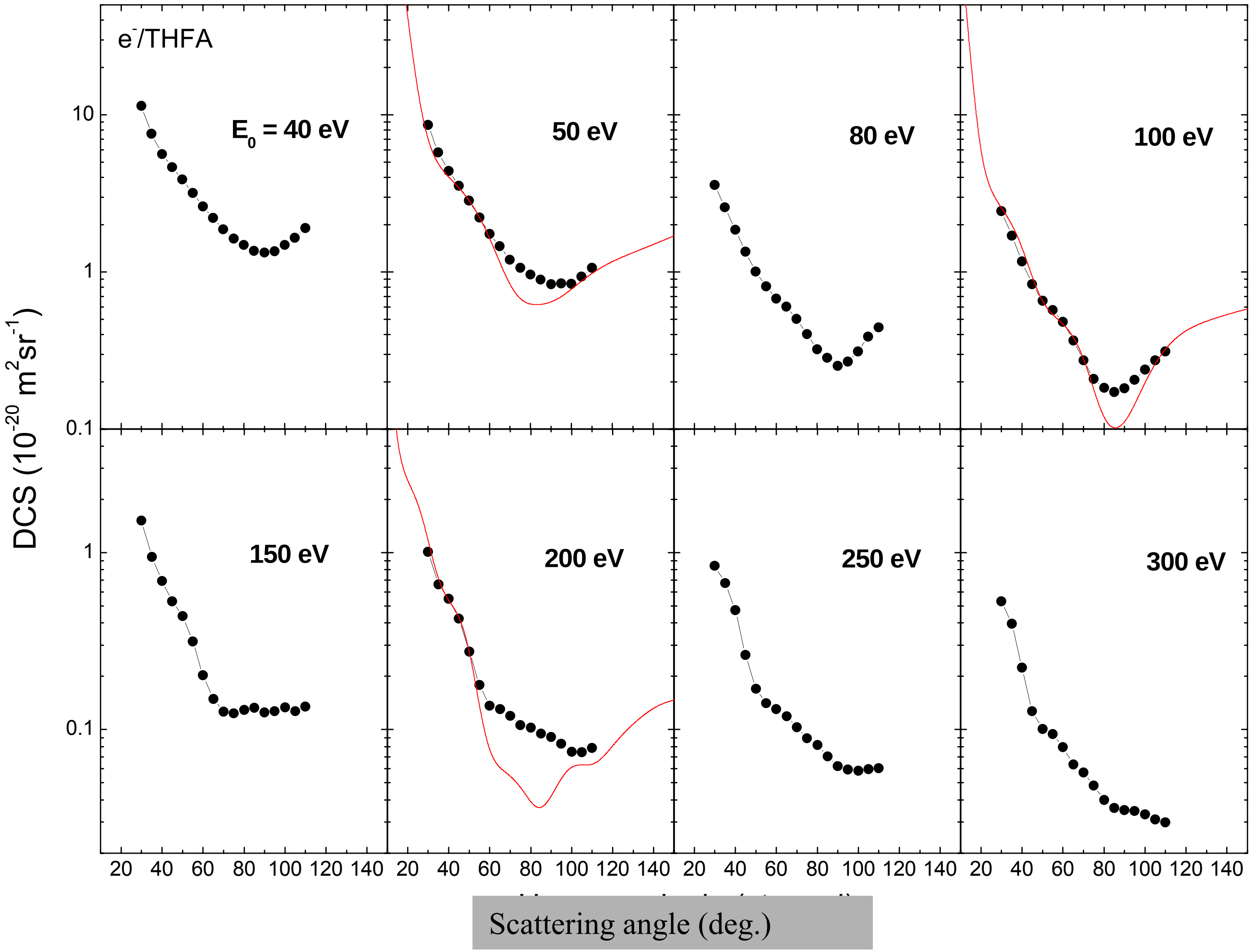
□,University of Liège and ●,Institute of Physics, Belgrade

Milosavljevic *et al* 2005 *Eur. J. Phys. D* **35** 411. *Ed.* E. Illenberger

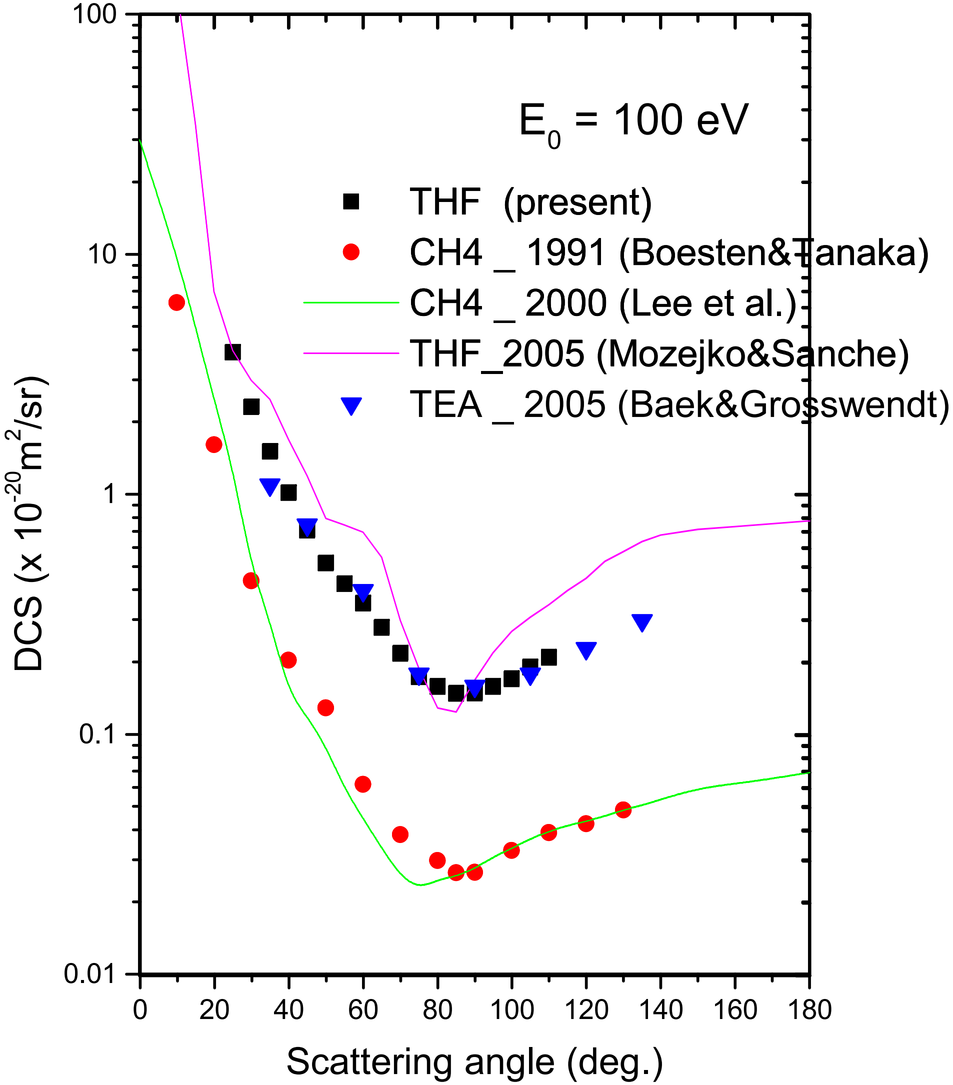


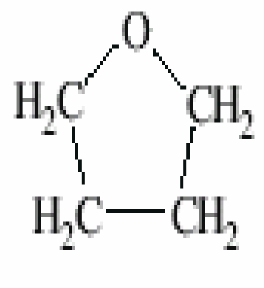
□,University of Liège and ●,Institute of Physics, Belgrade

Milosavljevic *et al* 2006 *Eur. J. Phys. D* to be submitted

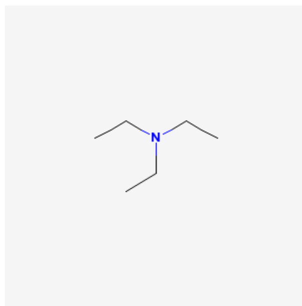


–, Mozejko and Sanche, calculations; ●,Institute of Physics, Belgrade

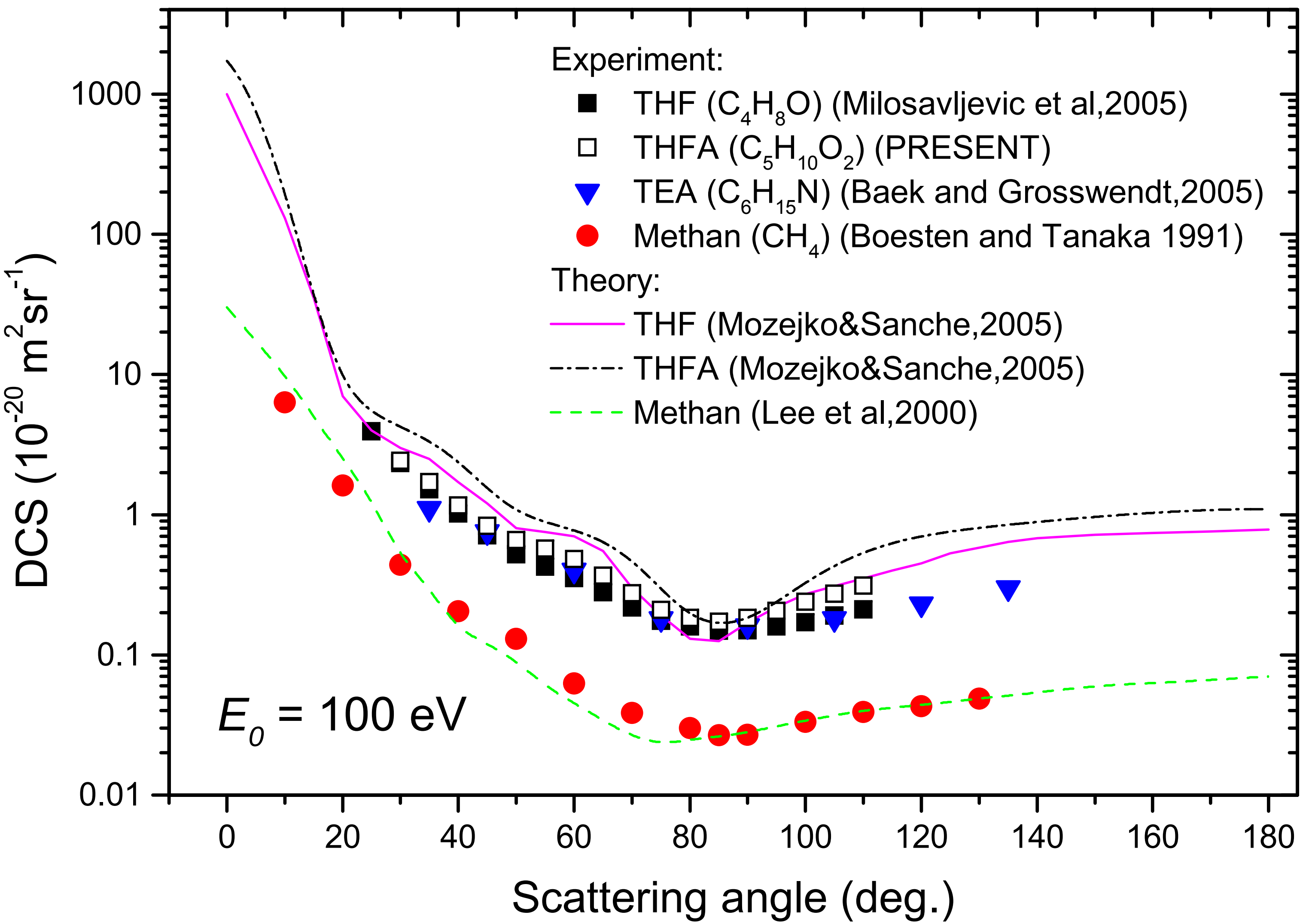




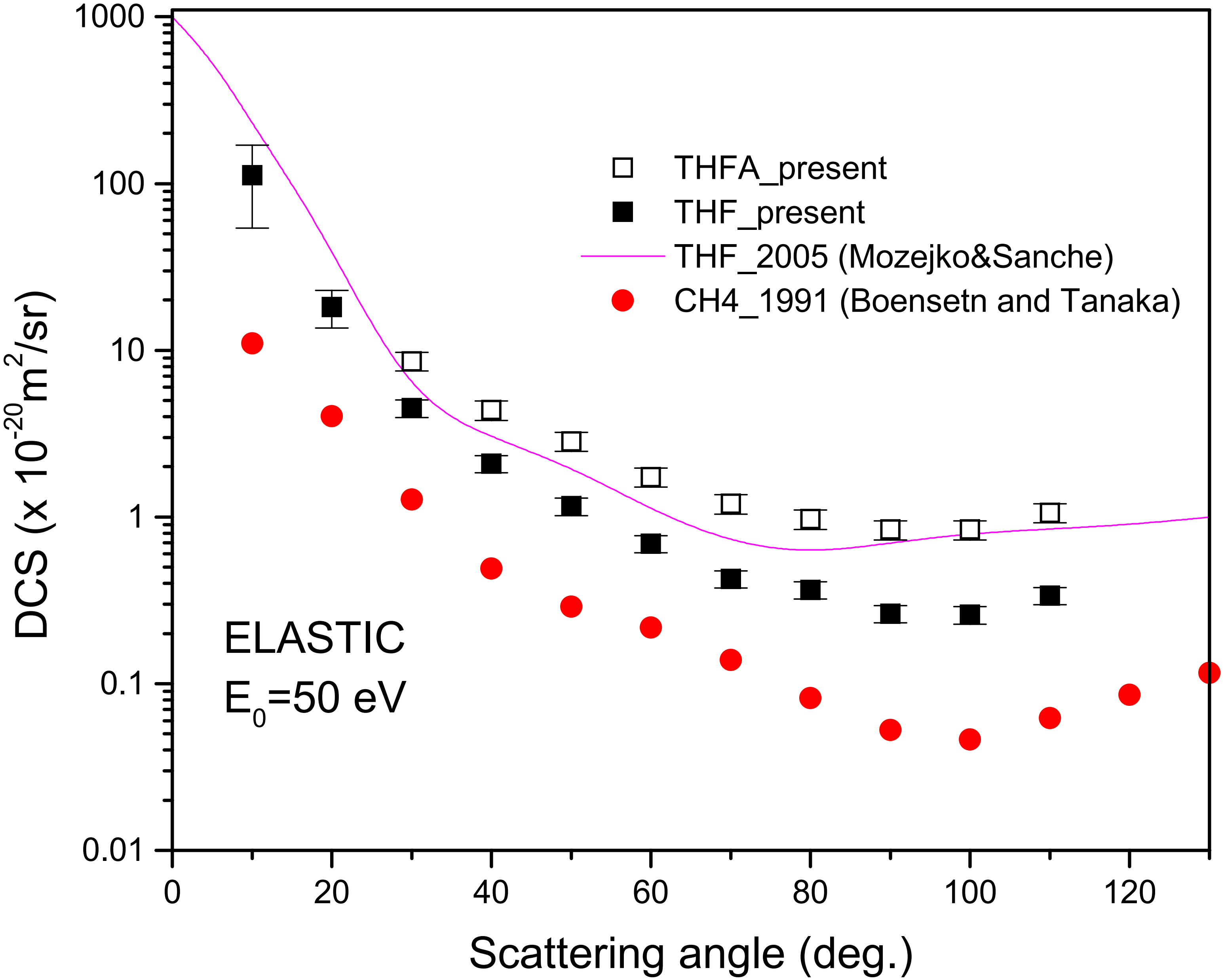
THF



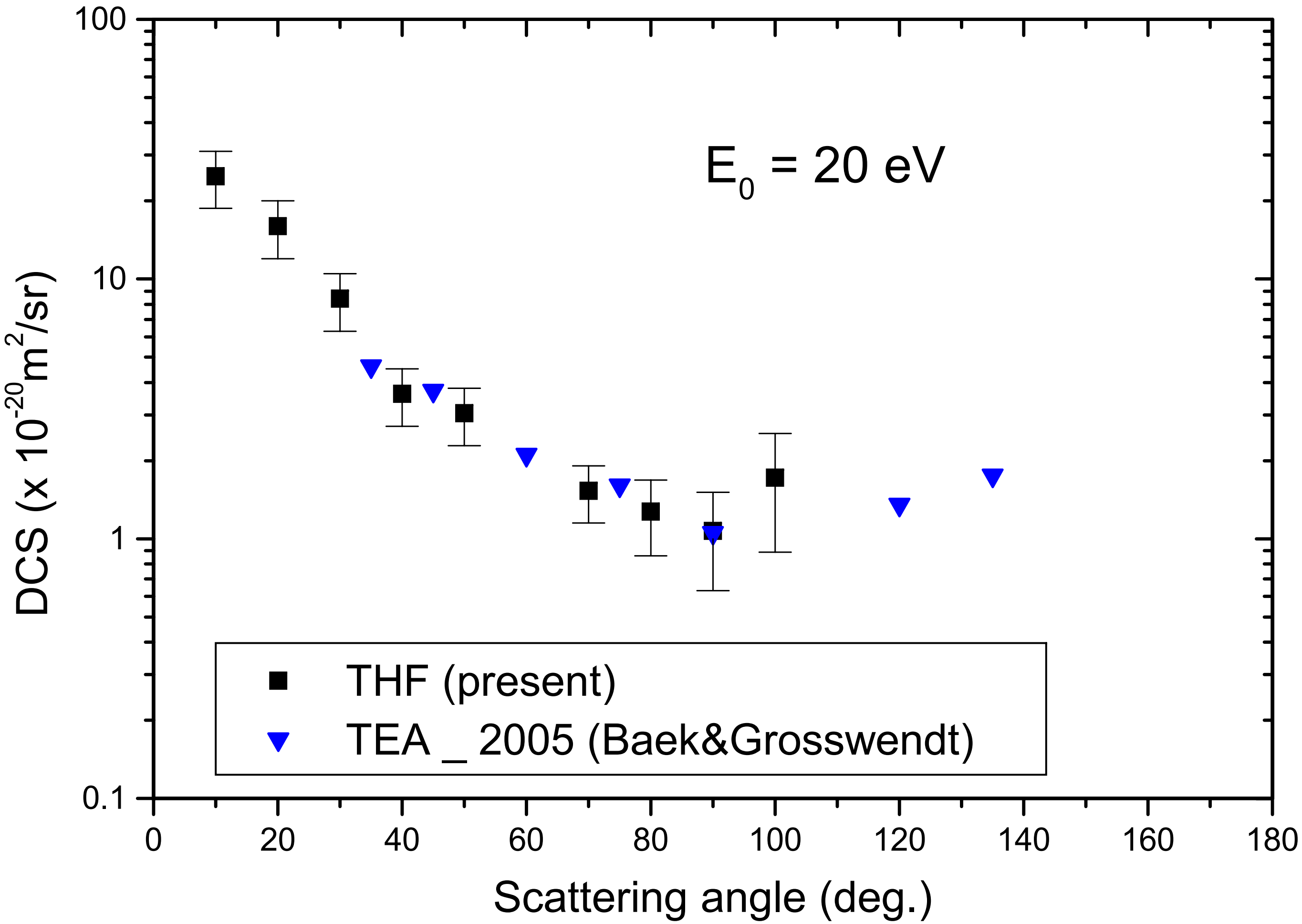
TEA-Triethylamine



Experiment:
THF (C_4H_8O) (Milosavljevic et al,2005)
THFA ($C_5H_{10}O_2$) (PRESENT)
TEA ($C_6H_{15}N$) (Baek and Grosswendt,2005)
Methan (CH_4) (Boesten and Tanaka 1991)
Theory:
THF (Mozejko&Sanche,2005)
THFA (Mozejko&Sanche,2005)
Methan (Lee et al,2000)
E_0 = 100 eV
DCS (10^{-20} m^2sr^{-1})
Scattering angle (deg.)
0.01
0.1
1
10
100
1000
0
20
40
60
80
100
120
140
160
180

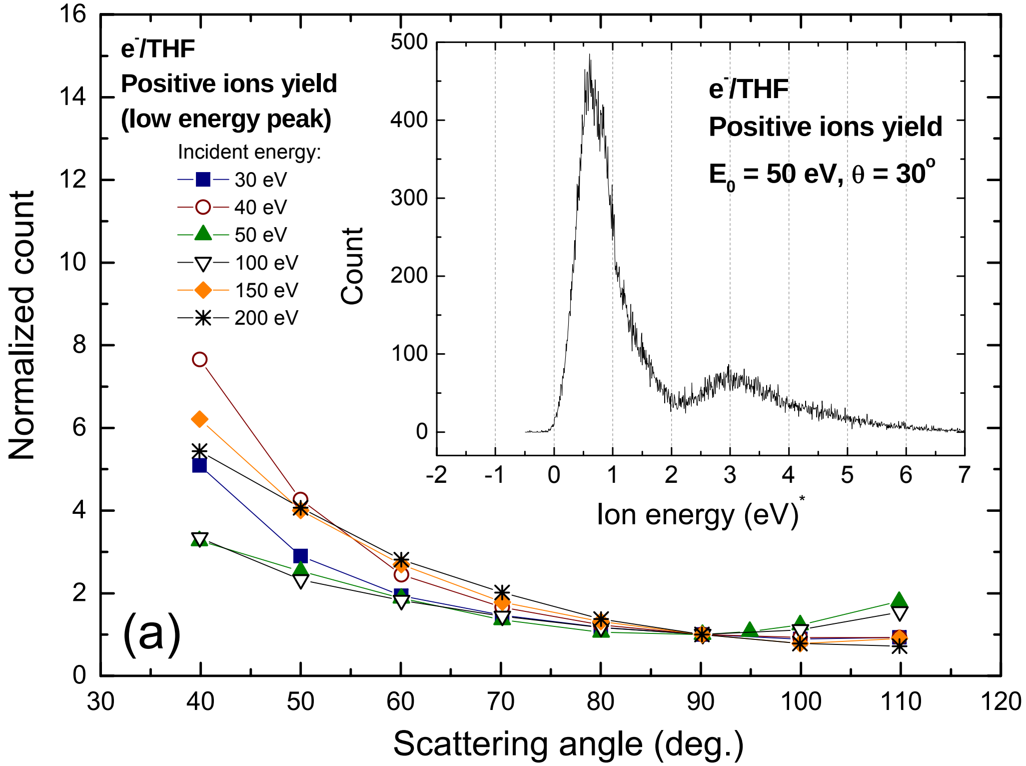


1000
100
10
1
0.1
0.01
DCS (x 10-20 m2/sr)
0
20
40
60
80
100
120
Scattering angle (deg.)
THFA_present
THF_present
THF_2005 (Mozejko&Sanche)
CH4_1991 (Boensetn and Tanaka)
ELASTIC
E0=50 eV


E0 = 20 eV
THF (present)
TEA _ 2005 (Baek&Grosswendt)
DCS (x 10-20m2/sr)
Scattering angle (deg.)
100
10
1
0.1
0
20
40
60
80
100
120
140
160
180

Electron induced dissociative ionization of THF

energy and angular distribution of positive ions



DEA

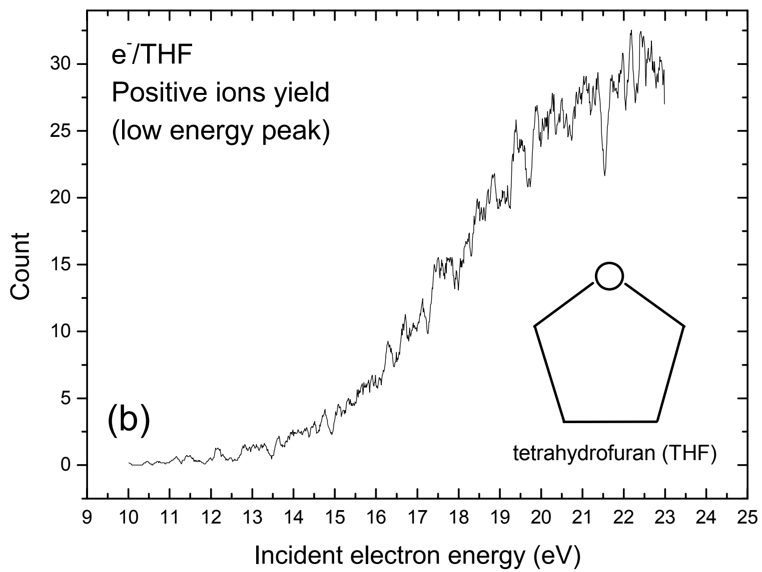
$$e^- + [R-H] \rightarrow [R-H]^- \rightarrow R^\bullet + H^-$$

DD resonant

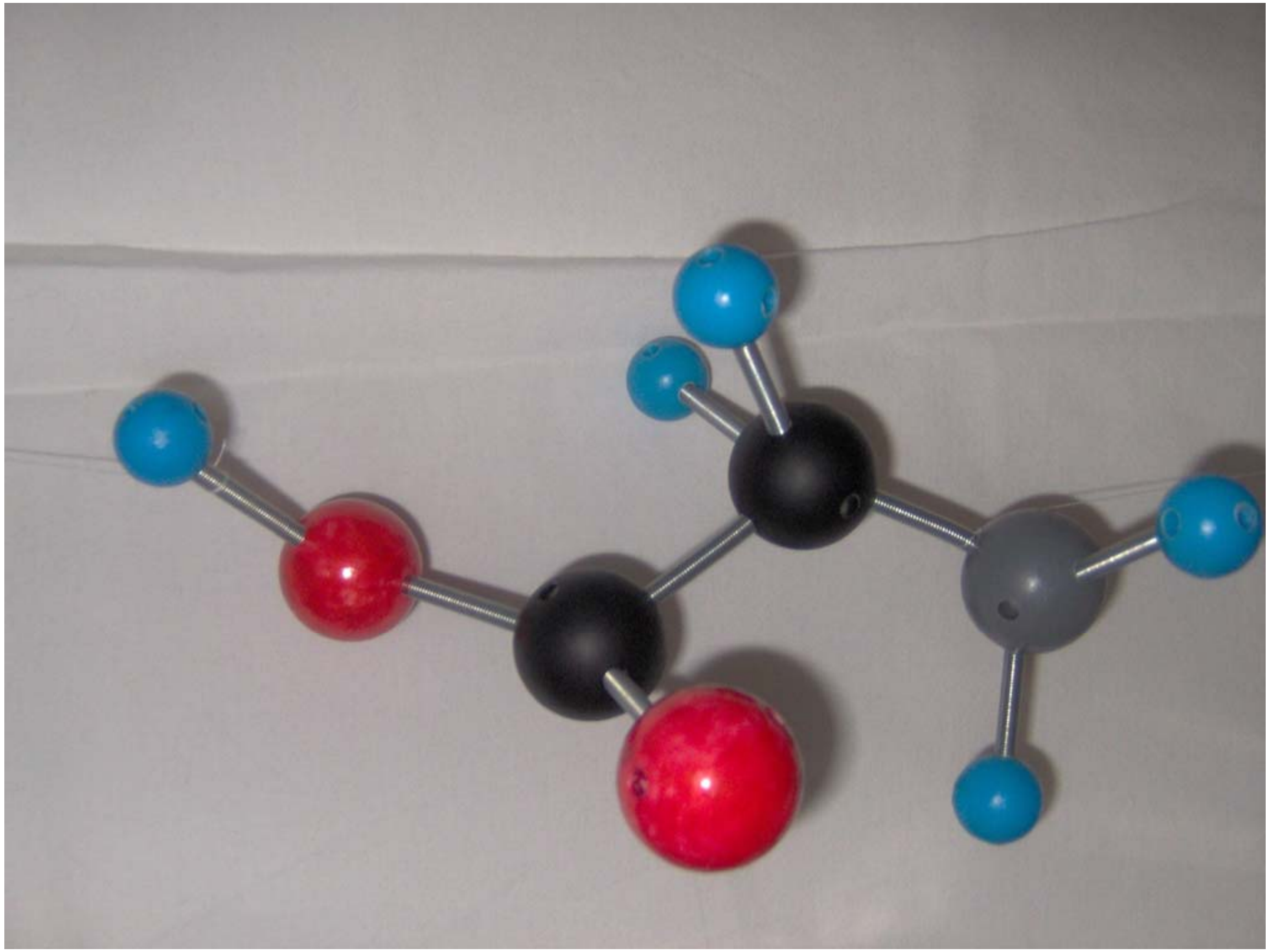
$$e + [R-H] \rightarrow [R-H]^- \rightarrow [R-H]^* + e \rightarrow R^+ + H^- + e$$

DD direct

$$e + [R-H] \rightarrow [R-H]^* + e \rightarrow R^+ + H^- + e$$

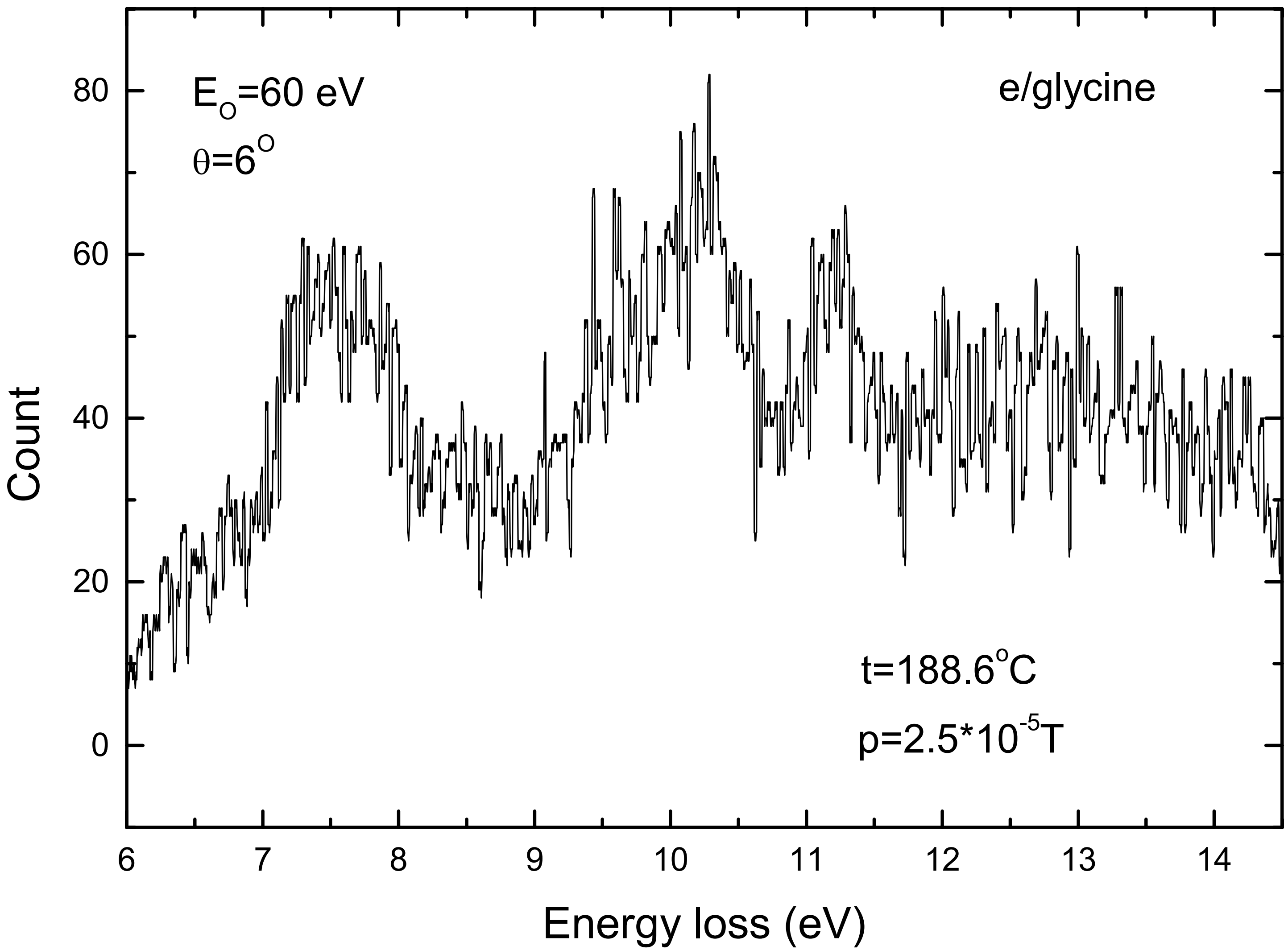


Glycine



$H_2N\text{-}CH_2\text{-}COOH$

Energy loss spectra Glycine



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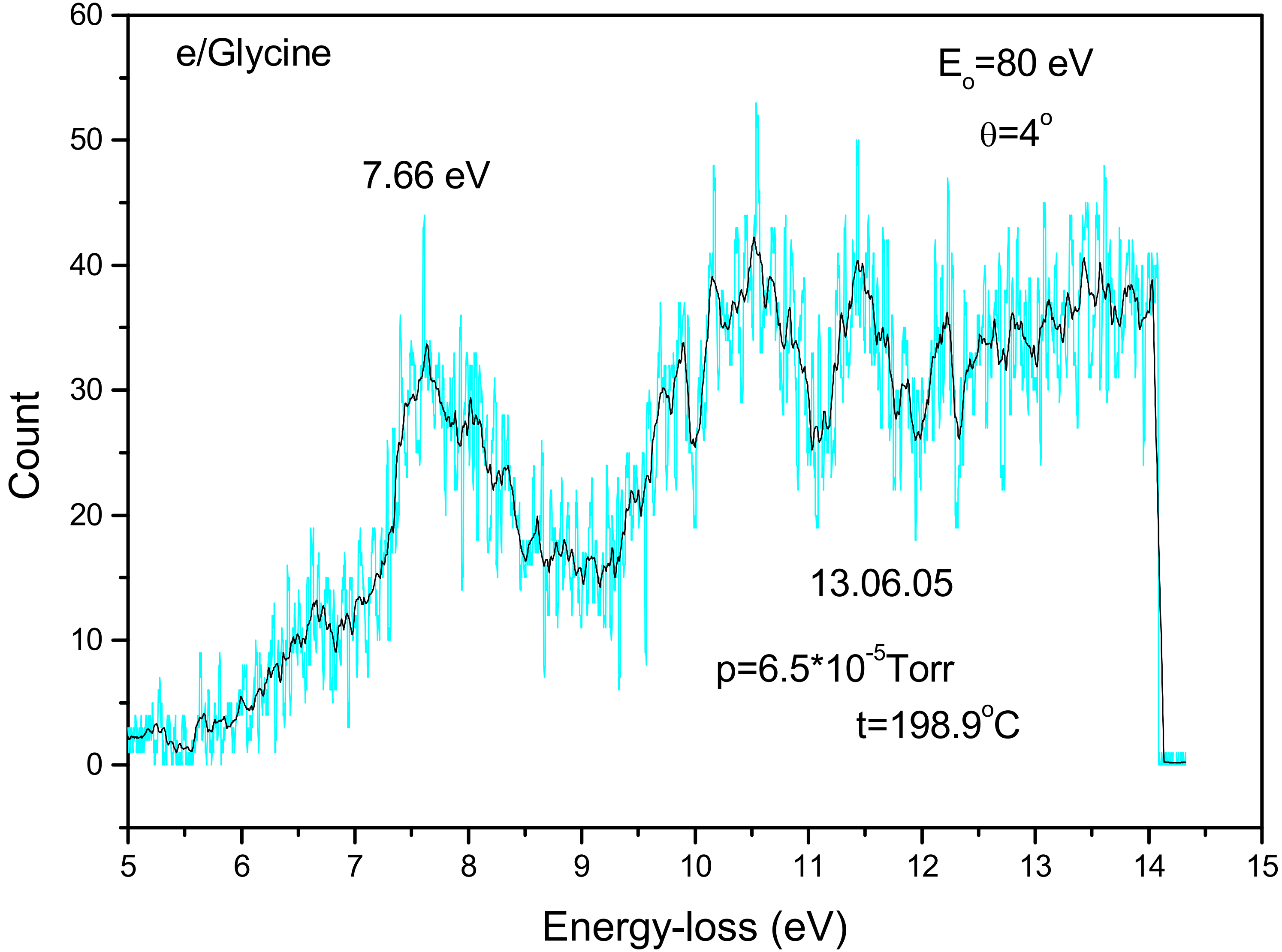
Energy loss spectra Glycine



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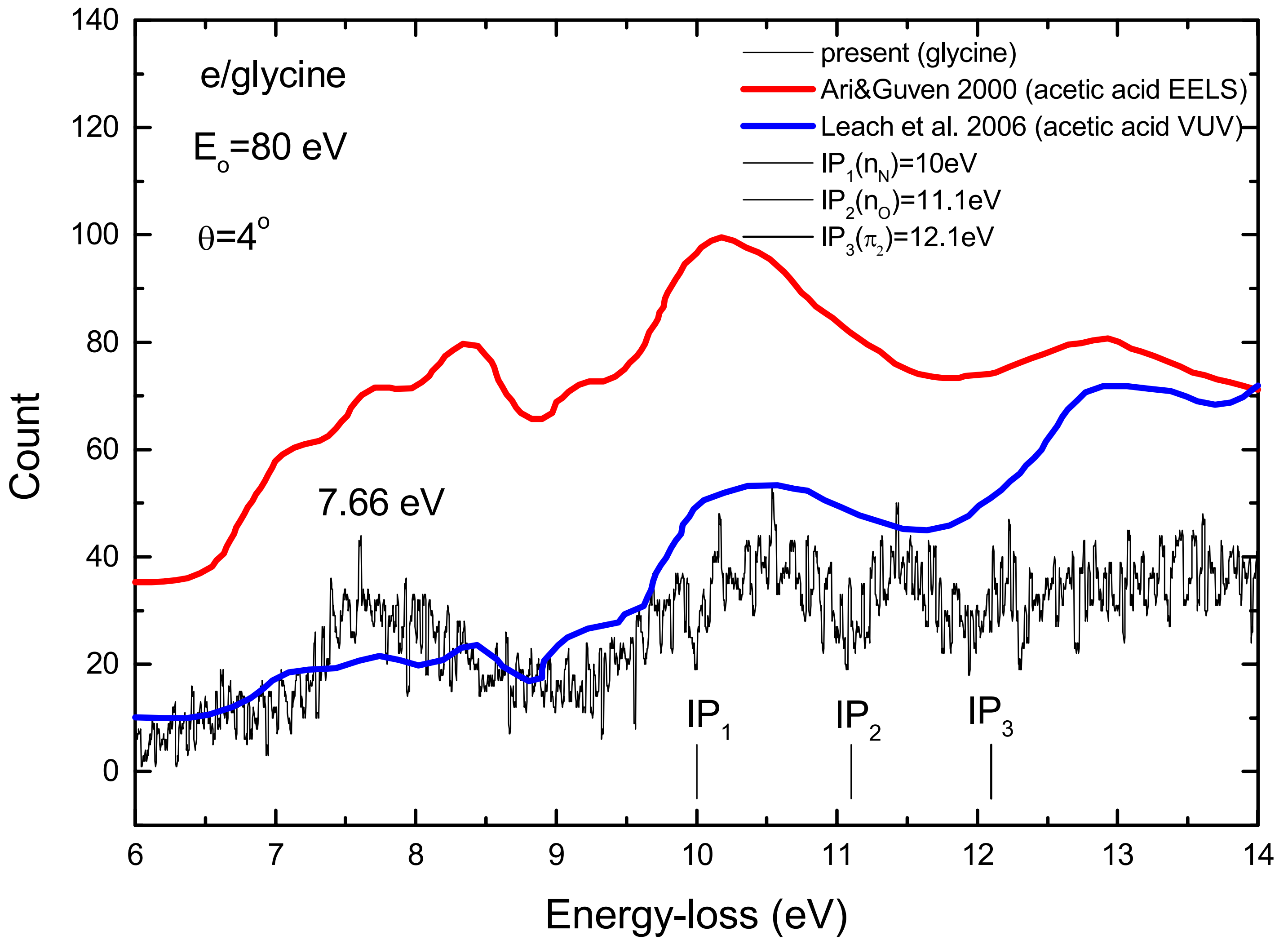
Energy loss spectra Glycine



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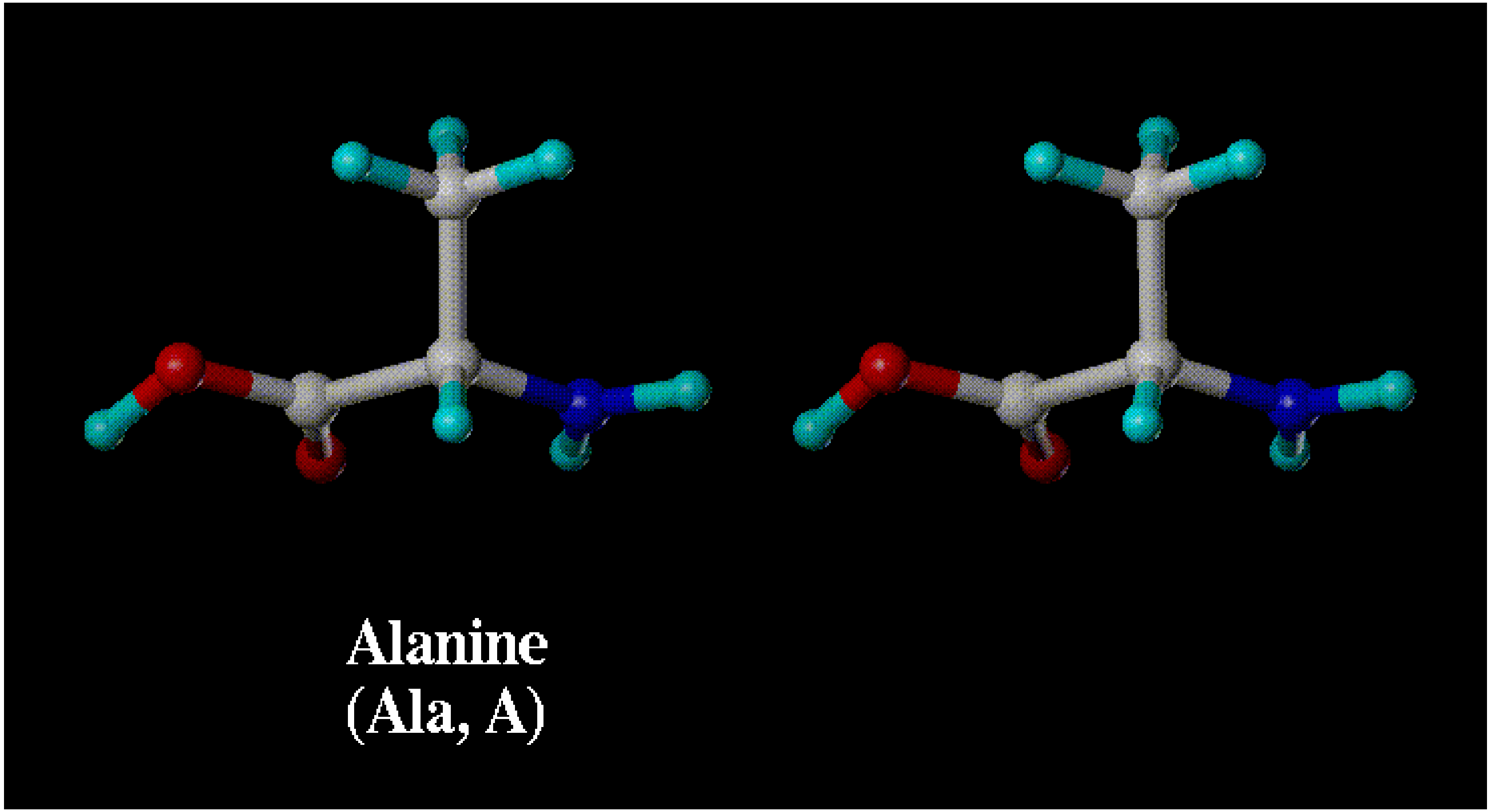
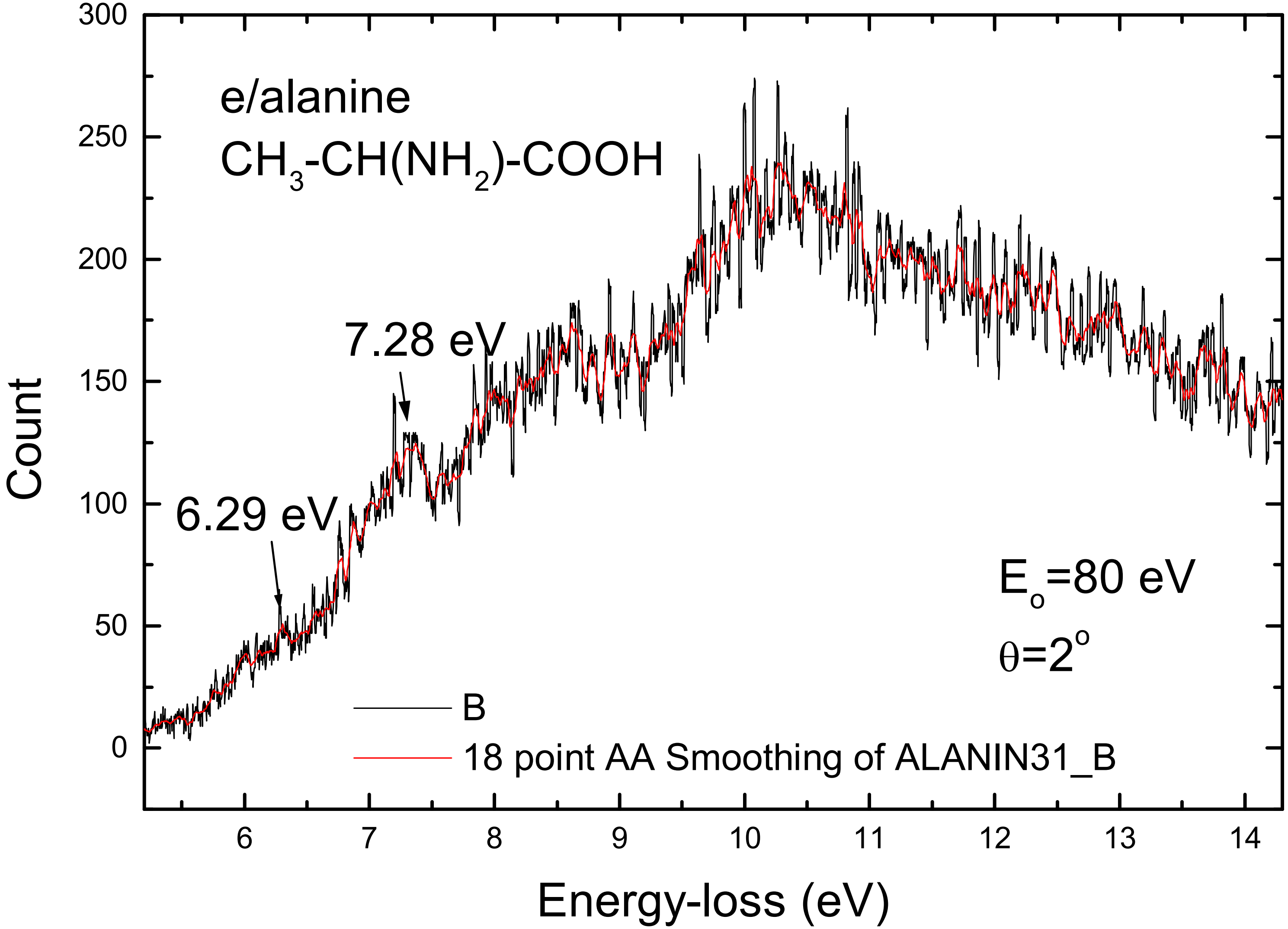
Energy loss spectra Alanine



CH_3-$CH(NH_2)$-$COOH$

Energy loss spectra Alanine



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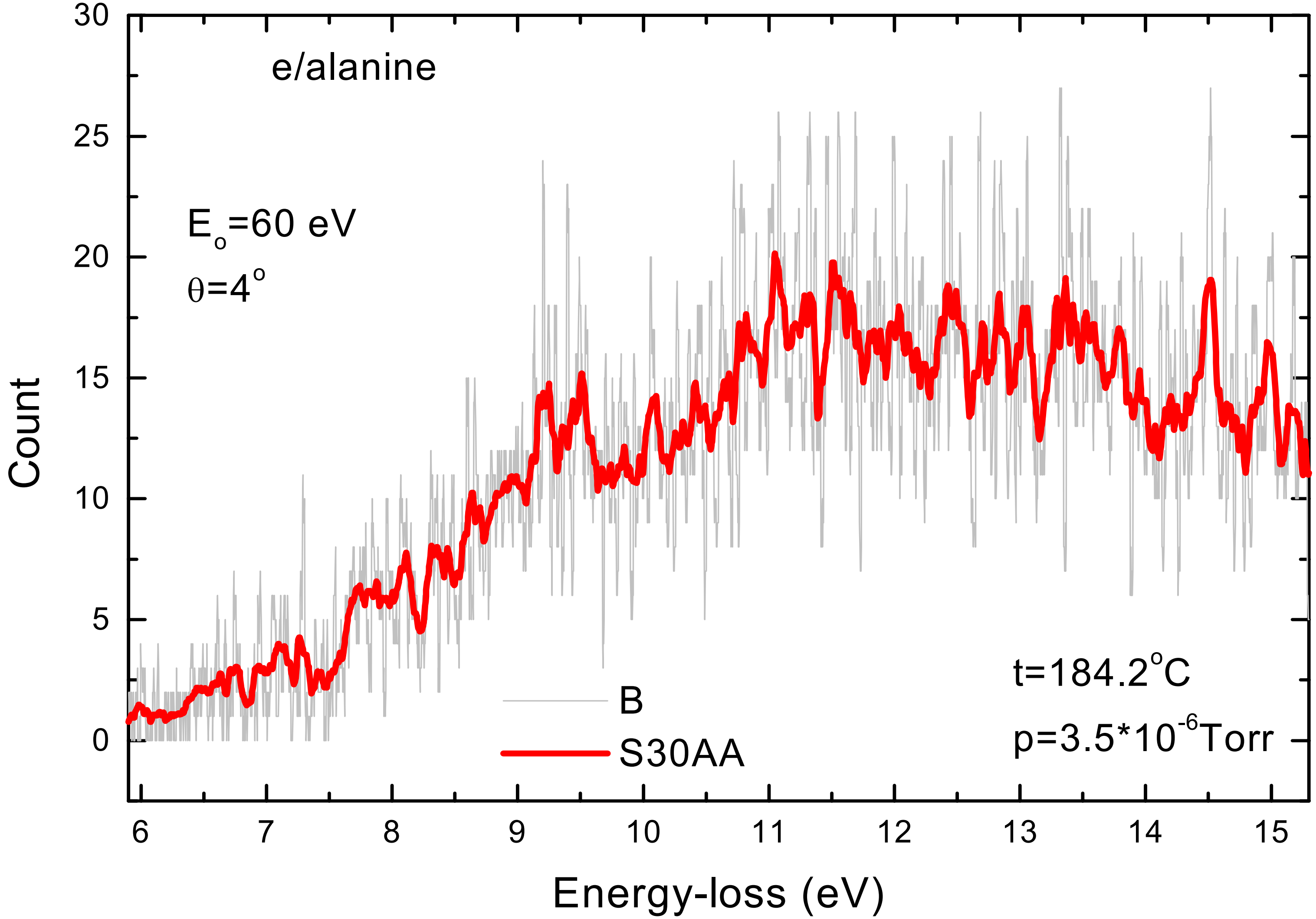
Energy loss spectra Alanine



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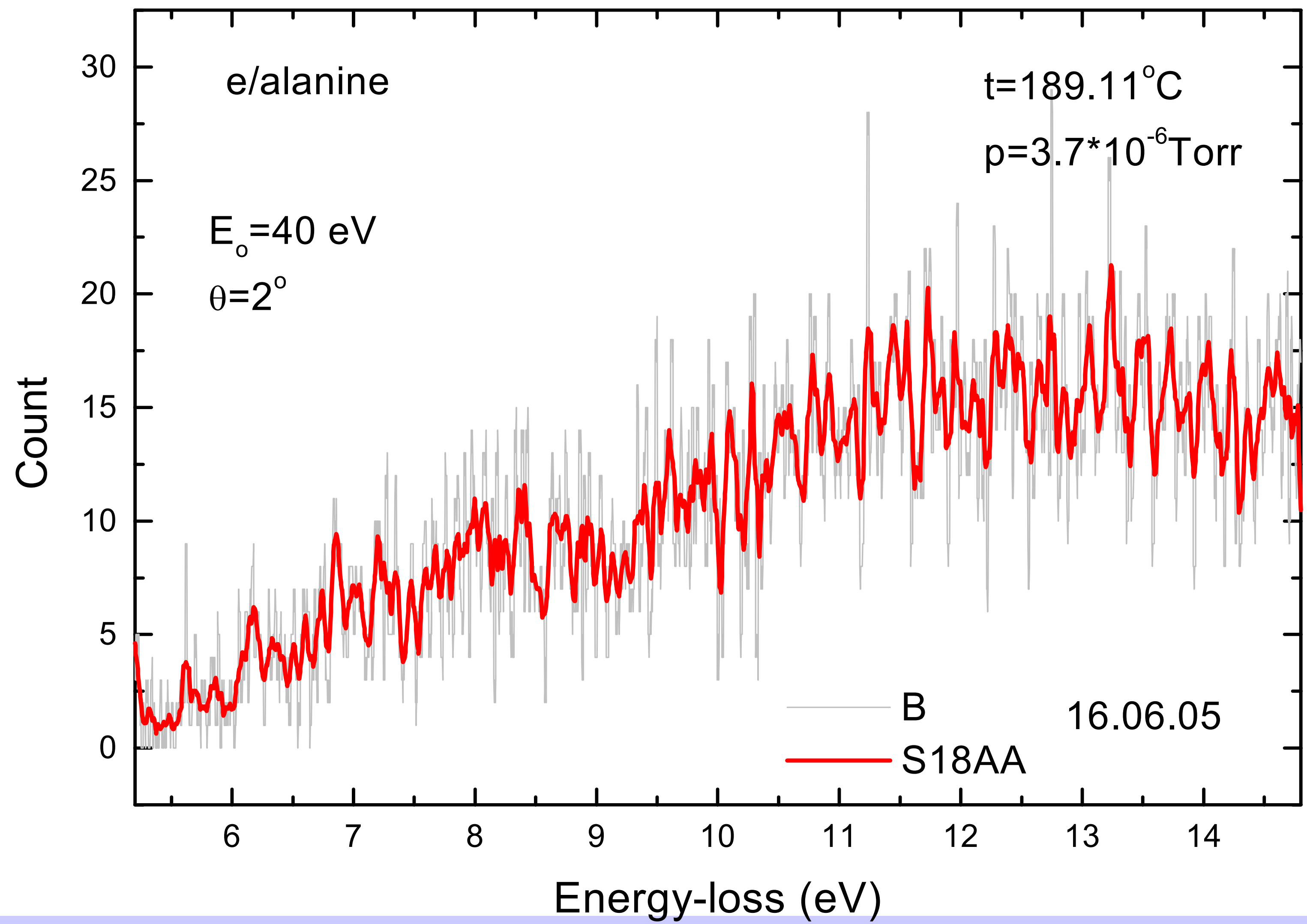
Energy loss spectra Alanine



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Questions:

1. *Why is it the first step towards understanding of basic interactions?*
2. *What we can learn from differential cross sections?*
3. *What is the relevance of data taken in binary collisions?*

Questions:

1. *Why is it the first step towards understanding of basic interactions?*

G. Garcia:

•Relevant for modeling of radiative energy deposition models;

•Pathway decisions: Differential elastic and inelastic collision cross sections required;

•Energy deposition in single collision: Experimental energy loss spectra needed.

Questions:

1. *Why is it the first step towards understanding of basic interactions?*

Barry D. Michael and Peter O'Neill:

•A clearer picture of the basic mechanisms (and potentially new chemical pathways) that induce DNA damage should also benefit the development of improved radiotherapy strategies for treating diseases such as cancer.

Questions:

2. What we can learn from differential cross sections?

- Compare absolute values and shapes;
- Create models for accurate calculations (from simple IAM-Independent Atom Model, complex optical potential models to R-matrix and ab-initio models;

Questions:

2. What we can learn from differential cross sections?

- Probe type of interaction (F A Gianturco:(i) the long-range nature of the charge-dipole interaction that mixes several channels over an usually large region of electron-molecule distances and (ii) the correct inclusion of the short-range contributions from exchange and polarization forces which alter rather drastically the anisotropy of the electronuclear forces within the molecular volume).

Questions:

3. What is the relevance of data taken in binary collisions?

- Put certain limits to the strength of interaction;
- Interactions could be smeared by the presence of the other molecules and aggregates;
- We need to start from the binary collisions to in order to understand radiative energy deposition and to include refined effects.

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the first step towards understanding of basic interactions

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Thank you for your attention!

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