ELASTIC ELECTRON SCATTERING ON THE ANESTHETIC MOLECULES IN THE GAS PHASE AT MEDIUM ENERGY RANGE

(joint experimental and theoretical study)

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Content

- Introduction: motivation, why anestetics, biomolecules, methane, Ar)
- Theory models
- Experimental set up: UGRA electron spectrometar
- Results
- Conclusion

Introduction

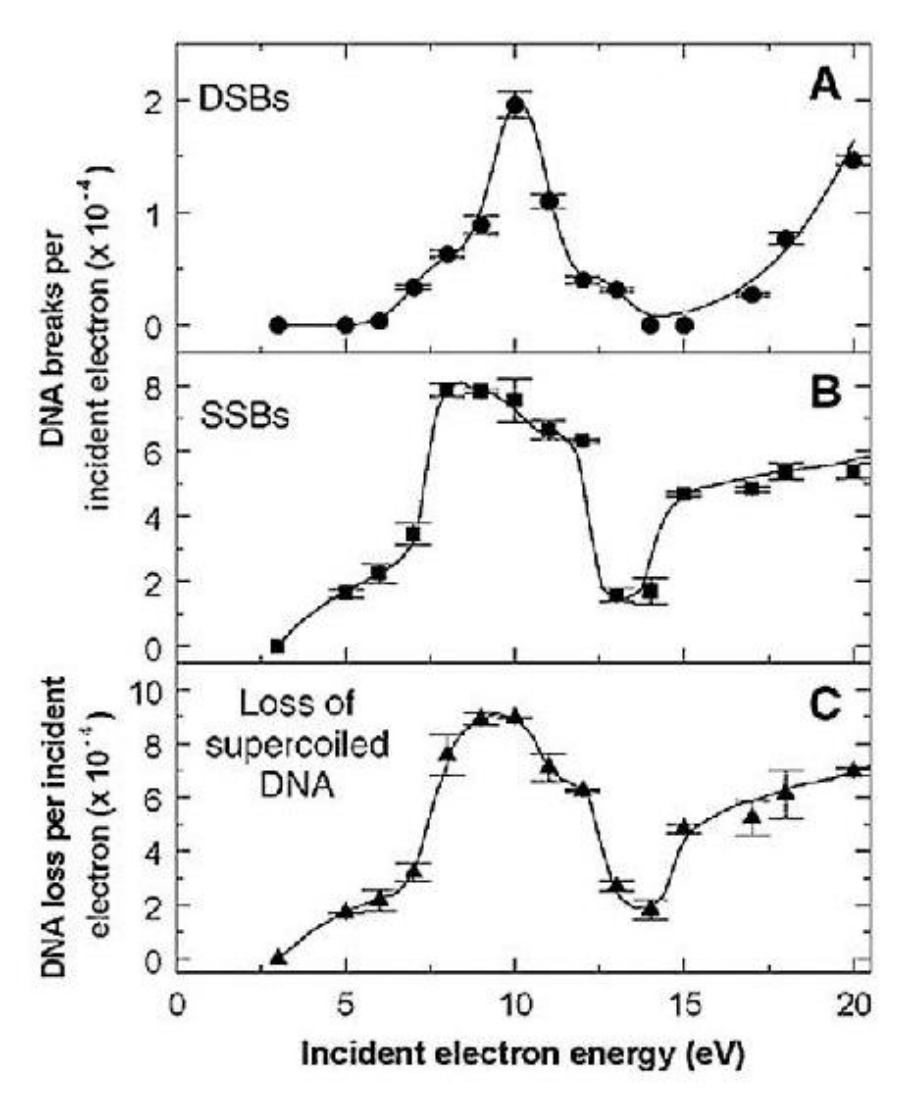
Why biomolecules – *radiation damage*

- High energy Ionization - breaks the strands in molecules
- a) particle: electrons, neutrons, protons..

  b) electromagnetic radiation: X and γ radiation
- Radiation damage - effects in living tisue which are product of high energy ionization (breaks the strands in biomolecule; SSB, DSB).
- Direct damage of biomolecules – high energy particle produces great nuber of secondary low energy electrons.
- The high-energy particle produces excited molecules, radicals, cations, anions and secondary electrons (SE) < 30 eV
- Large number of SE ~ 10^5/MeV carry most of the deposited energy
- Secondary low energy electrons (3-20 eV) damage DNA

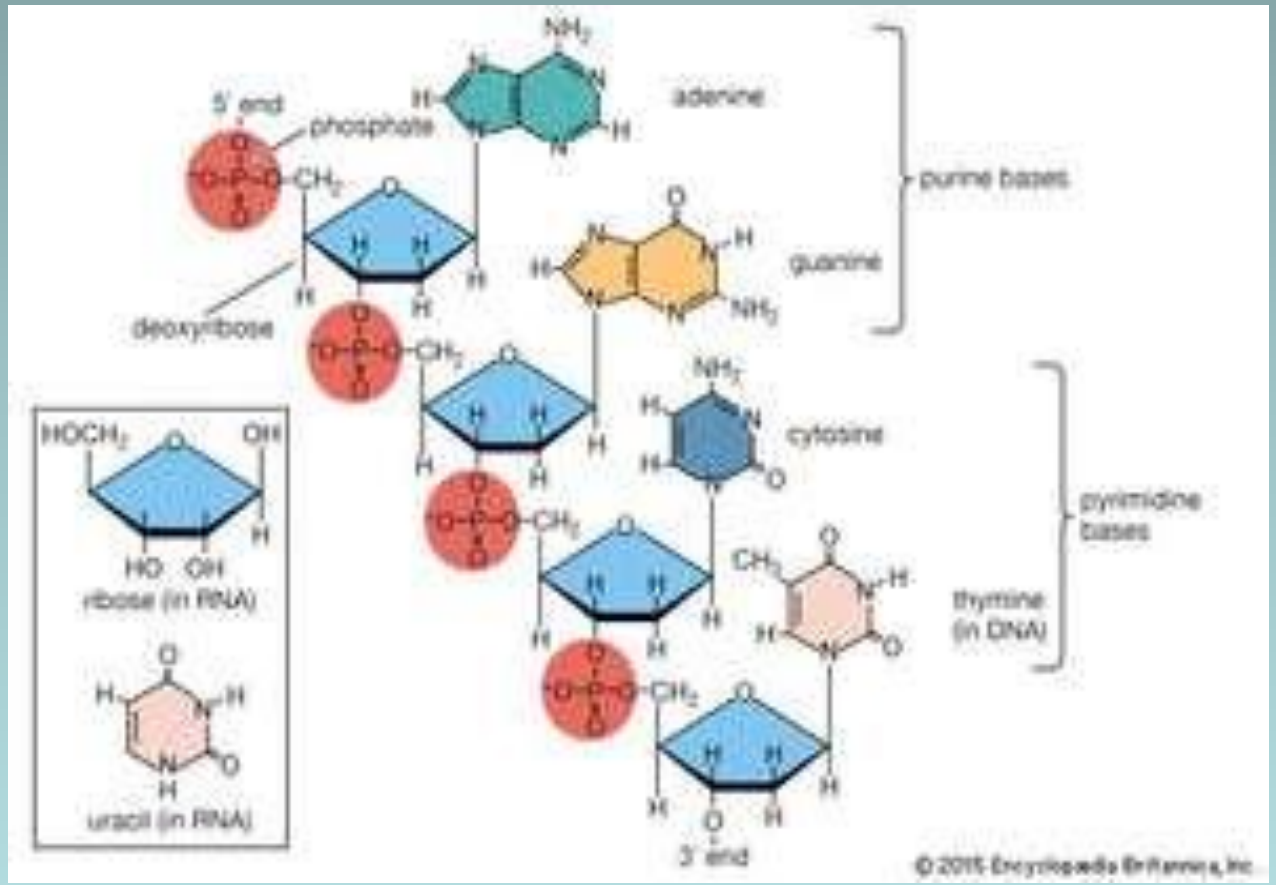
  (***Boudaiffa et al, Science 287 , 2000***)

Inspiration for the research

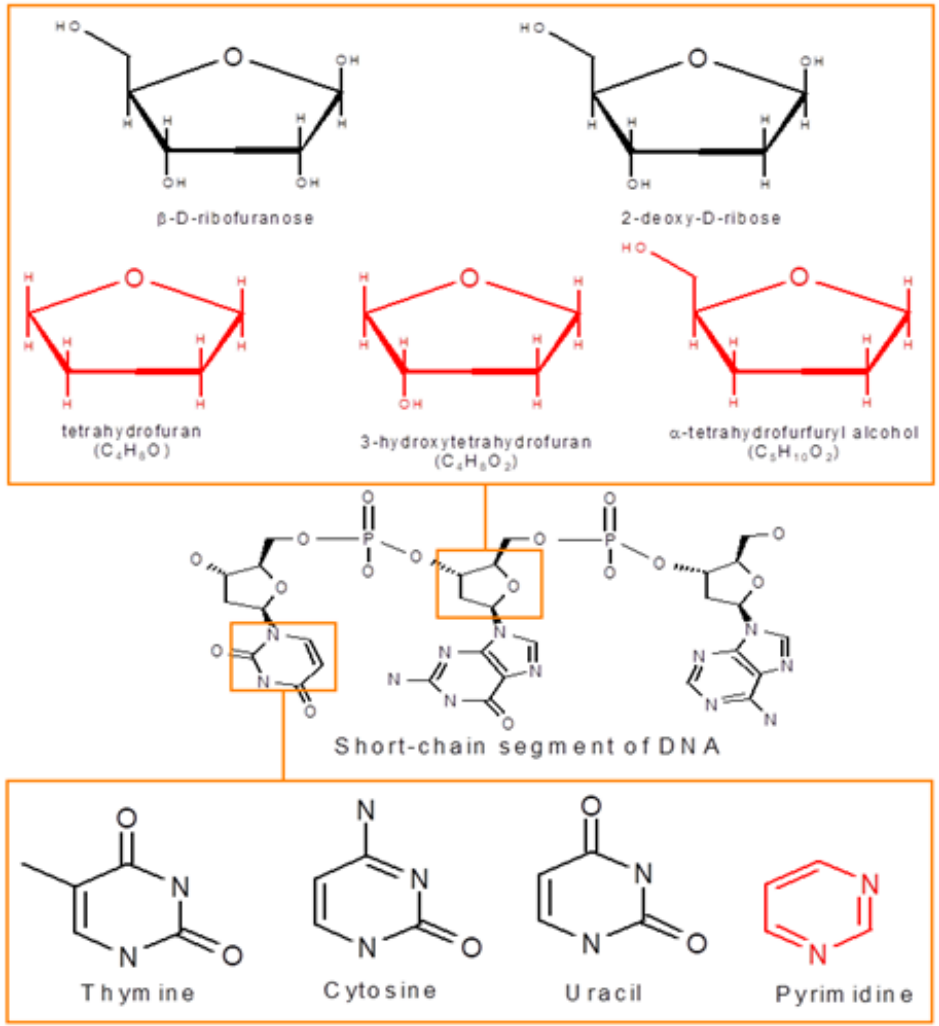


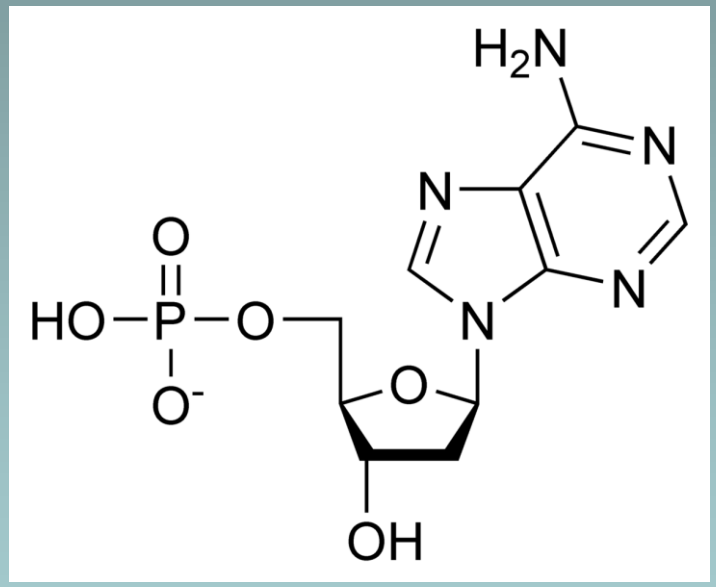
B. Boudaiffa et al Science 287, 1658 (2000).

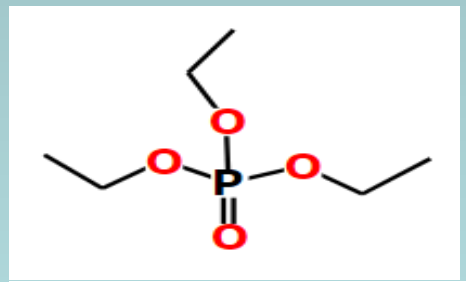
DNA molecule



Investigated biomolecules



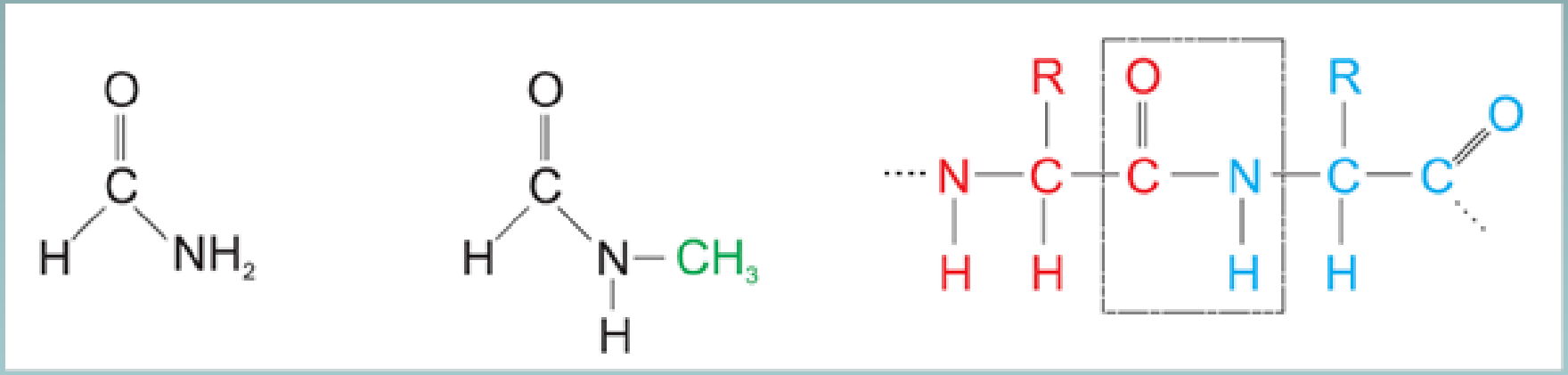




Triethyl phosphate (TEP)

$C_6H_{15}O_4P$

Investigated molecules



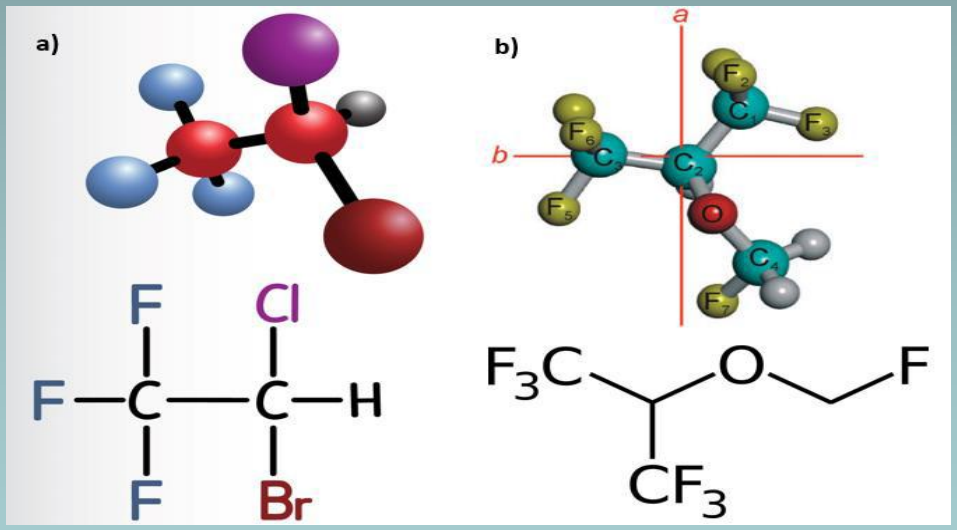
Formamide N-metilformamid Peptide bond

Why aneasthetics

- Fluorinated compounds are of particular interest due a wide range of applications from medicine to modern technology materials.
- Impact on the environment has motivated further research
- Most of the inhaled aneaesthetics are eliminated from the patient's body without being metabolized, so they are released into the lower atmosphere
- Its tropospheric lifetime is calculated to be 7 years (Langbein et al. 1999), long enough to reach the stratosphere in considerable quantities. There, halothane can damage the ozone layer, since its ozone depletion potential (ODP) is 1,56 (Langbein et al. 1999), highest among all aneaesthetics.
- Halothane is known to have a high global warming potential

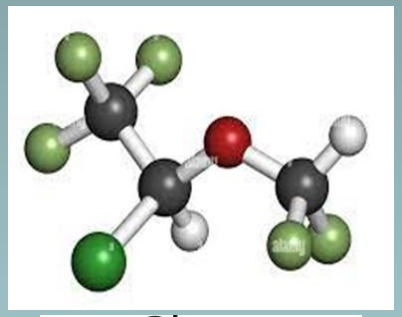
Investigated anaesthetics

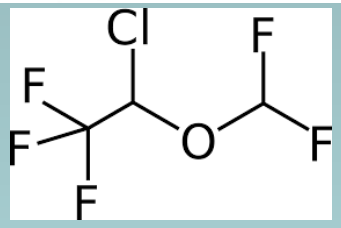
Halothane



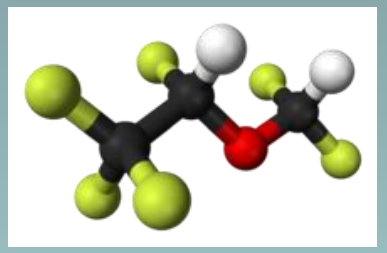
Sevoflurane

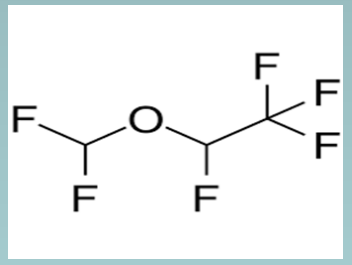
Isoflurane





Desflurane





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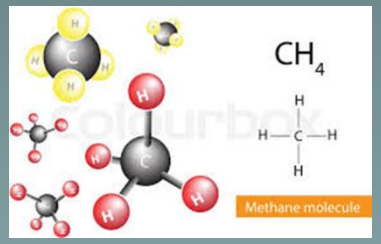
Investigated molecule methane, motivation



- Methane (CH_4) is the simplest hydrocarbon molecule and has attracted significant interest as a target for energy electron collision studies.
- Major component of the atmosphere of the outer planets (Jupiter, Saturn, Uranus, Neptune) and their satellites
- Present in plasma technologies, e.g. plasma synthesis of diamonds
- Methane is one of the most prevalent long-lived greenhouse gases (together with carbon dioxide and nitrous oxide).
- It has many technological and atmospheric applications as well as a fundamental importance as one of the testing grounds for the collision theories.
- Because the abundance of this strong greenhouse gas is growing, it is important to understand its interaction mechanism with other molecules, atoms and particles, including electrons.

Theory

Theory models

Electron-atom interaction can be approximated with optic potential:

$$V_{opt}(r) = V_s(r) + V_e(r) + V_p(r) + iV_a(r)$$

$$f(\theta) = \frac{1}{2ik}\sum_{l=0}^{l\max}(2l+1)(e^{2i\delta l} - 1)\rho_l \cos(\theta)$$

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2$$

- **I**ndependent **A**tom **M**odel – **IAM**

$$\sigma^{molecule} = \frac{4\pi}{k}\,\mathrm{Im}\,F(\theta = 0) = \frac{4\pi}{k}\sum_{atoms}\mathrm{Im}\,f_i(\theta = 0) = \sum_{atoms}\sigma^{atom}$$

- **S**creen **C**orrected **A**dditivity **R**ule (**SCAR**) : $\sigma^{tot} = \sum_i S_i\sigma_i$
- **SCARN:** reduces contribution of interering terms on small scattering angle
- **SCARND:** calculate cross sections for rotational excitations, important for molecules with high dipol moment
- Calculations for Ar have been done using Mot's cross section for electron atom scattering $\frac{d\sigma}{d\Omega} = |f(\theta)|^2 + |g(\theta)|^2$

Theory models - Calculation of ratio vibrational/elastic cross sections

First Born Aproksimation-FBA

$$f(\overrightarrow{k_{out}} \leftarrow \overrightarrow{k_{in}}) = -4\pi^2 < \overrightarrow{k_{out}}|T|\overrightarrow{k_{in}} > \approx -4\pi^2 < \overrightarrow{k_{out}}|V|\overrightarrow{k_{in}} >$$

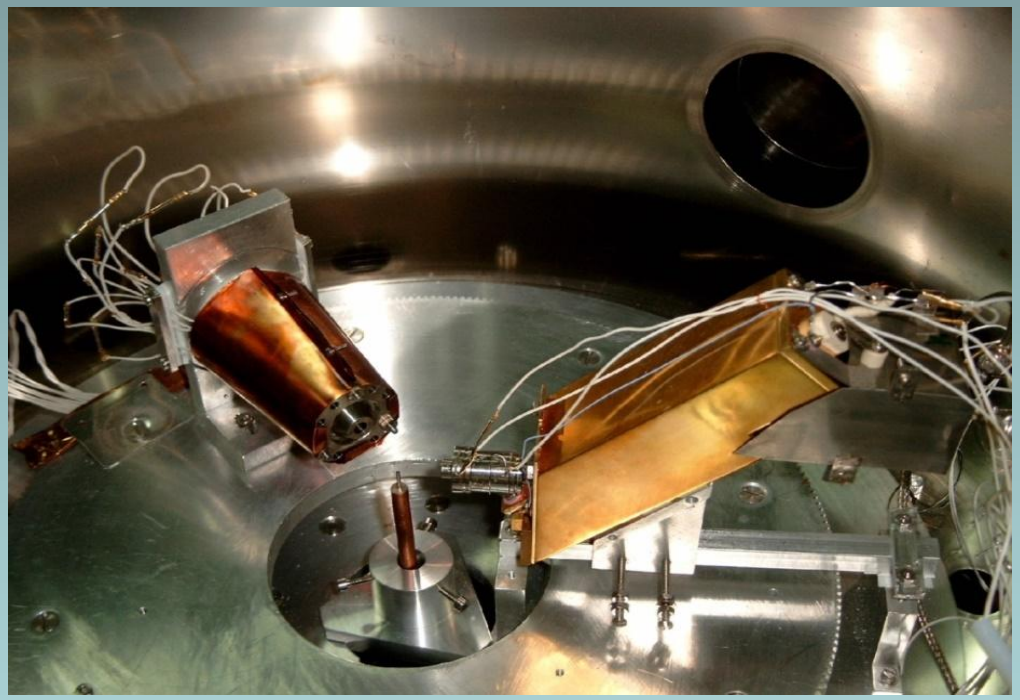
$$< \overrightarrow{k_{out}}|K|\overrightarrow{k_{in}} > \approx -\pi < \overrightarrow{k_{out}}|V|\overrightarrow{k_{in}} >$$

Unitarized First Born Aproksimation-FBA

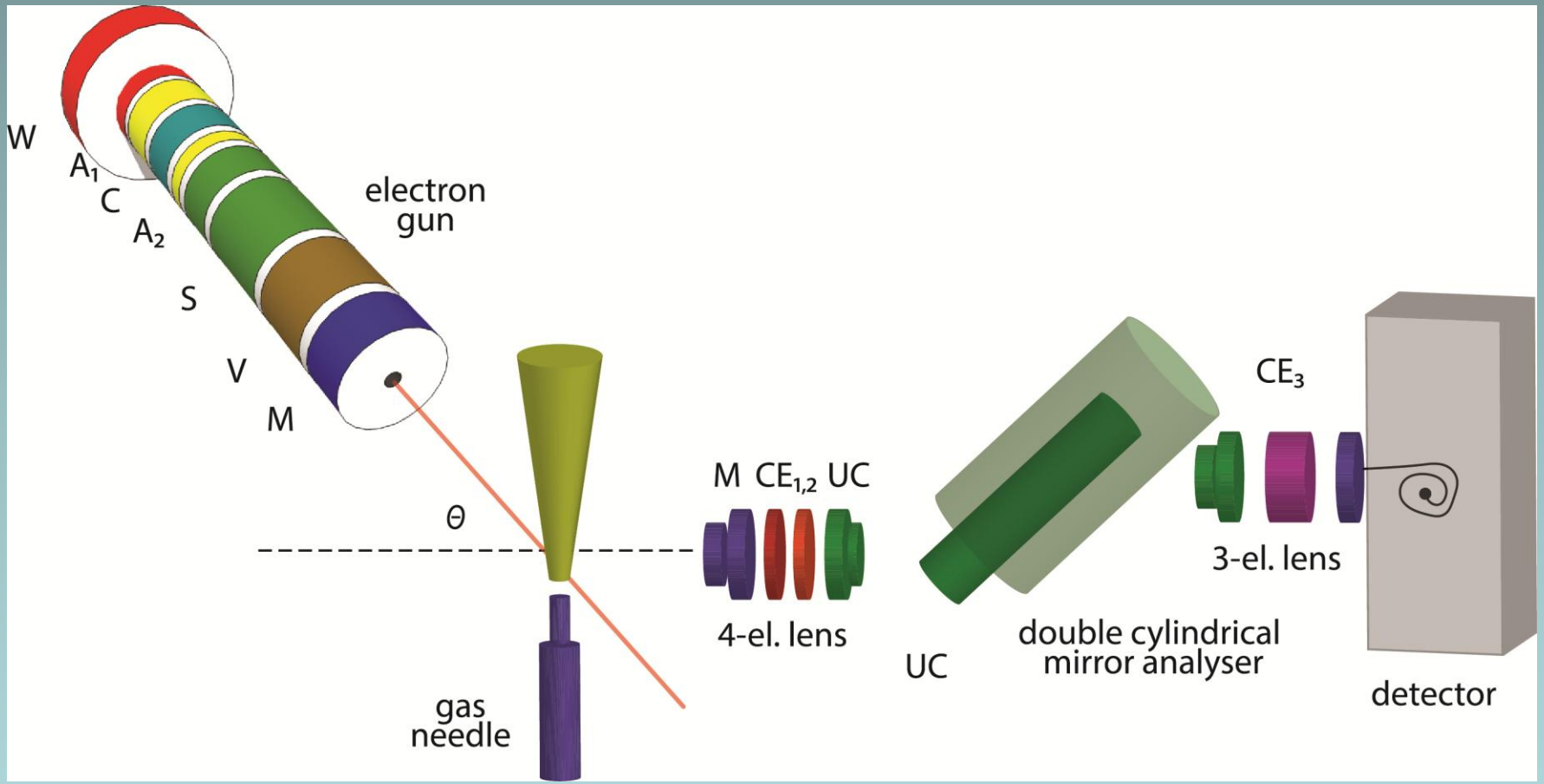
$$f_u(\overrightarrow{k_{out}} \leftarrow \overrightarrow{k_{in}}) = -4\pi^2 < \overrightarrow{k_{out}}|T_U|\overrightarrow{k_{in}} >$$

Experiment

Apparatus UGRA –experimental set up



- Angular resolution ±1,5^{o}
- Energy resolution 0.5 eV
- Basic pressure 5x10-7 mbar


W
A1
C
A2
S
V
M
electron
gun
Θ
gas
needle
M CE1,2 UC
4-el. lens
UC
CE3
3-el. lens
double cylindrical
mirror analyser
detector

Apparatus UGRA – *modes of operations*

- Relative differential cross sections – in function of scattering angle
- Relative differential cross sections – in function of incident electron energy
- Absolute differential cross sections-Relative flow method
- Spectra of kinetic energy distribution of positive ions
- Electron energy loss spectra

Test measurements for Ar

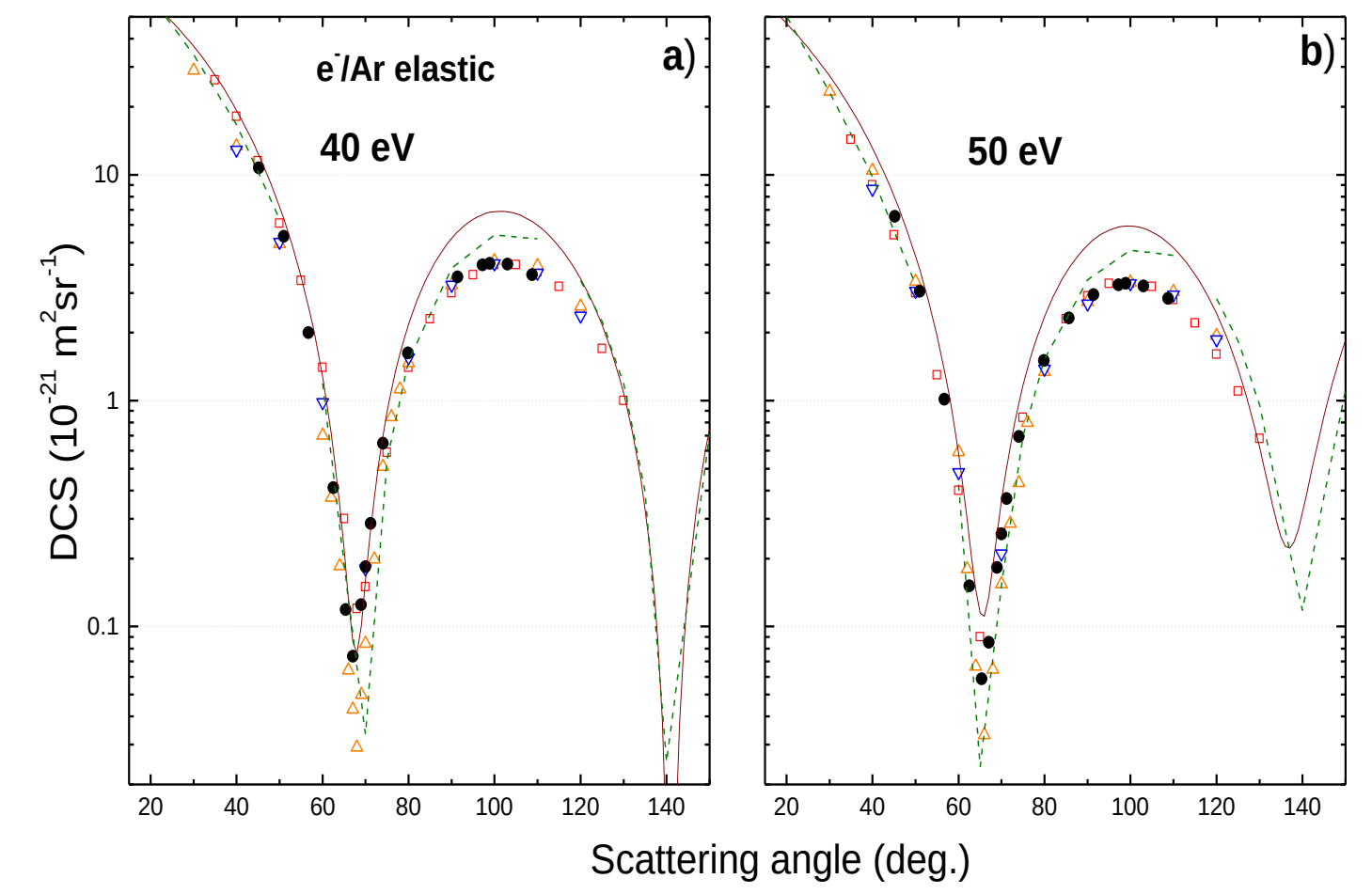
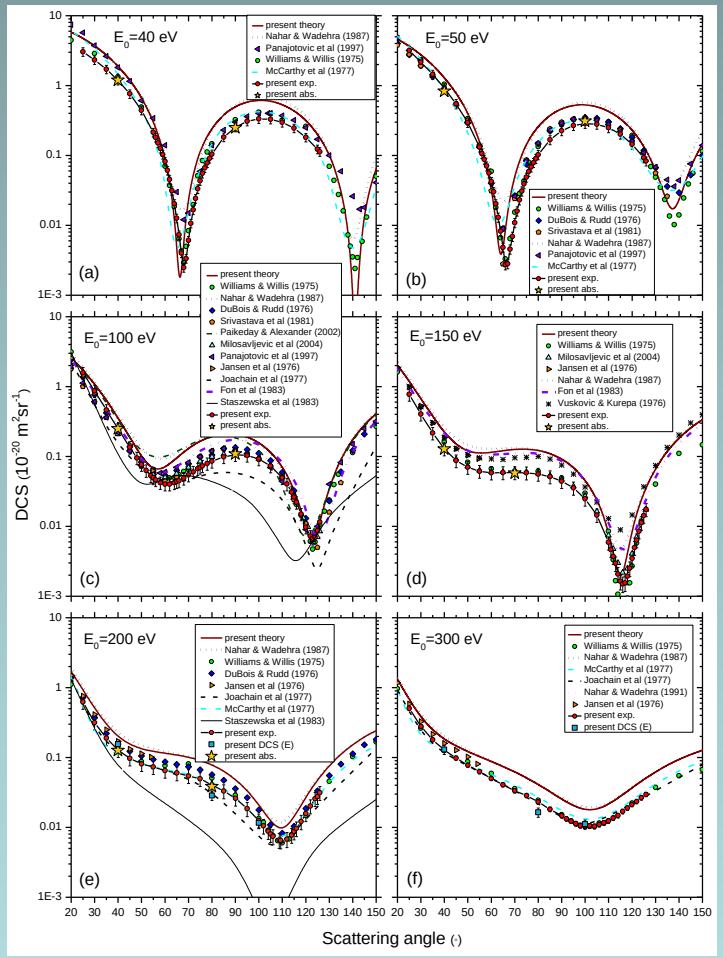


Fig. *The angle dependent DCSs for elastic electron-argon scattering at 40 eV (a) and 50 eV (b): present, ●; Panajotović et al 1997, □; Cvejanović and Crowe 1997, ▽; Srivastava et al 1981, ▼; Vušković and Kurepa 1976, *; Williams and Willis 1975, △; Sienkiewicz et al 2000, ——; Fon et al 1983, – –.*

ELASTIC SCATTERING – *absolute DCSs*

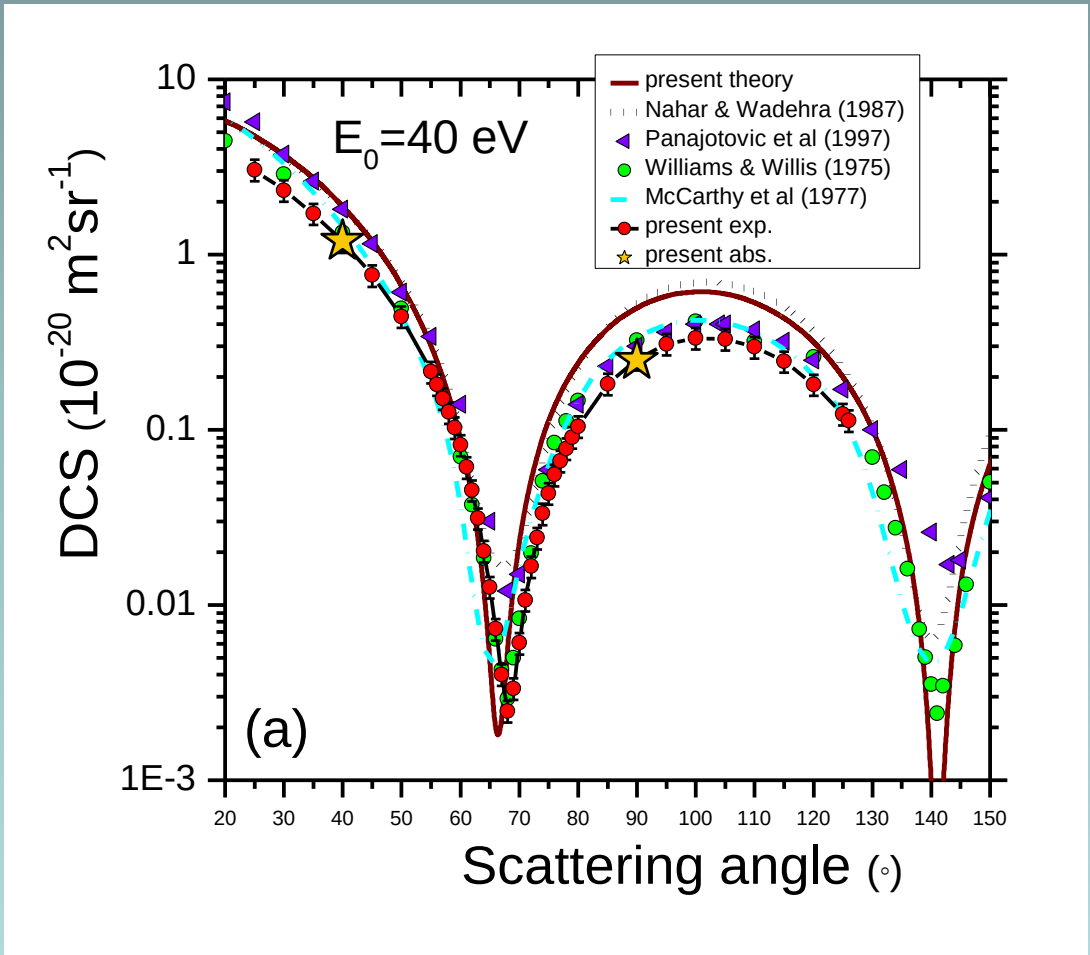
Ar(as a function of scattering angle)



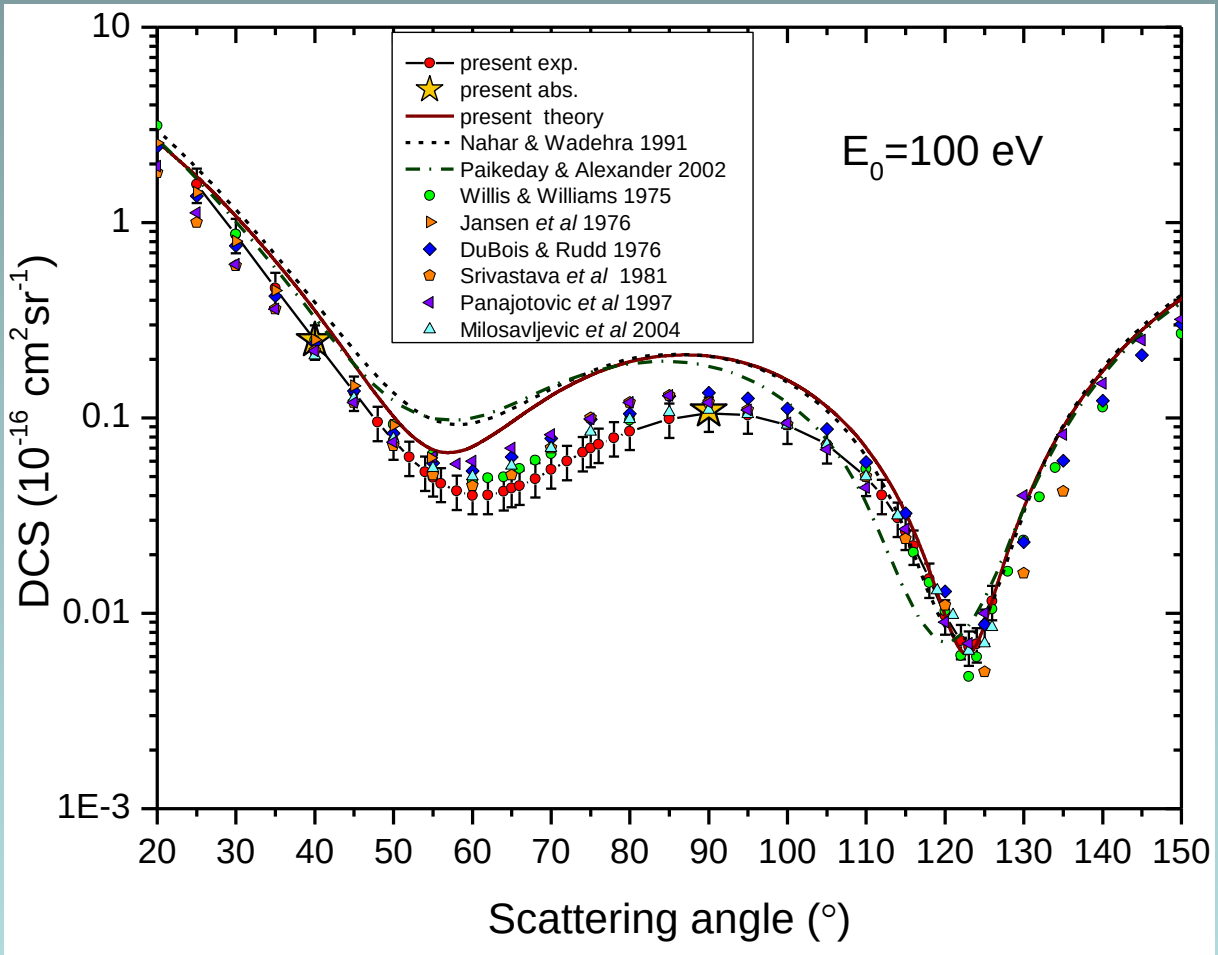
Ranković, Maljković et al Eur. Phys. J. D (2018) 72

ELASTIC SCATTERING – *absolute DCSs*

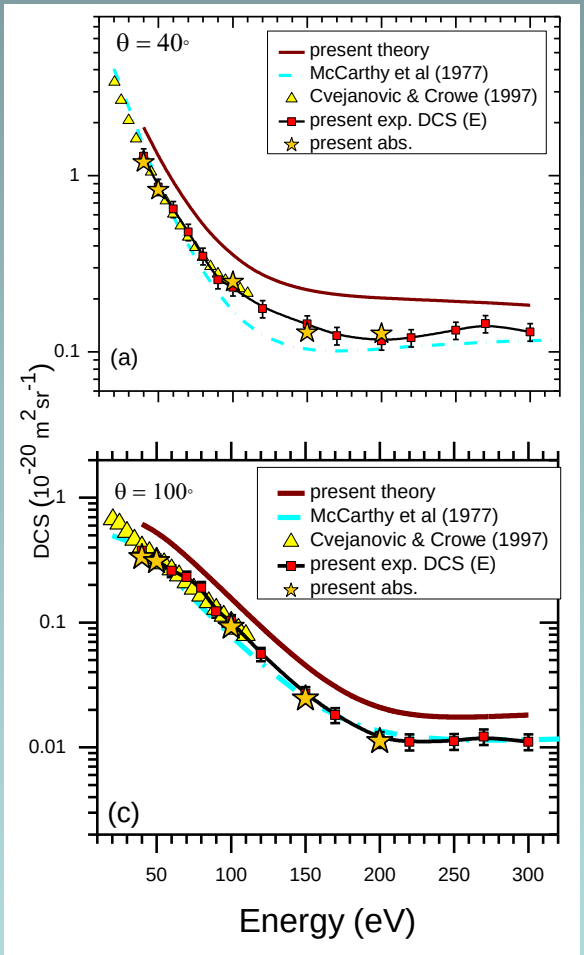
Ar, 40eV (as a function of scattering angle)



ELASTIC SCATTERING – *absolute DCSs*
Ar, 100eV(as a function of scattering angle)



ELASTIC SCATTERING – *absolute DCSs*
Ar (as a function of incident electron energy)



Measurement of relative DCSs

$$I(E_0,\theta) = DCS(E_0,\theta)\eta(E_0)V_{eff}(E_0,\theta)$$

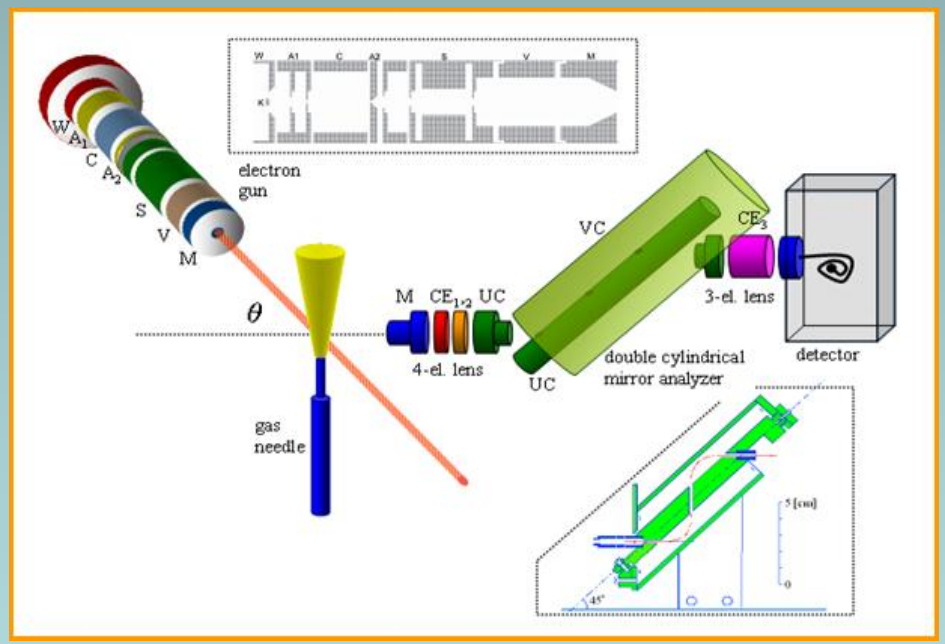
$$V_{eff} = \int \rho(r) f(r) \Delta\Omega(r) G[\theta(r)] dr$$

Relative DCSs in the function of scattering angle

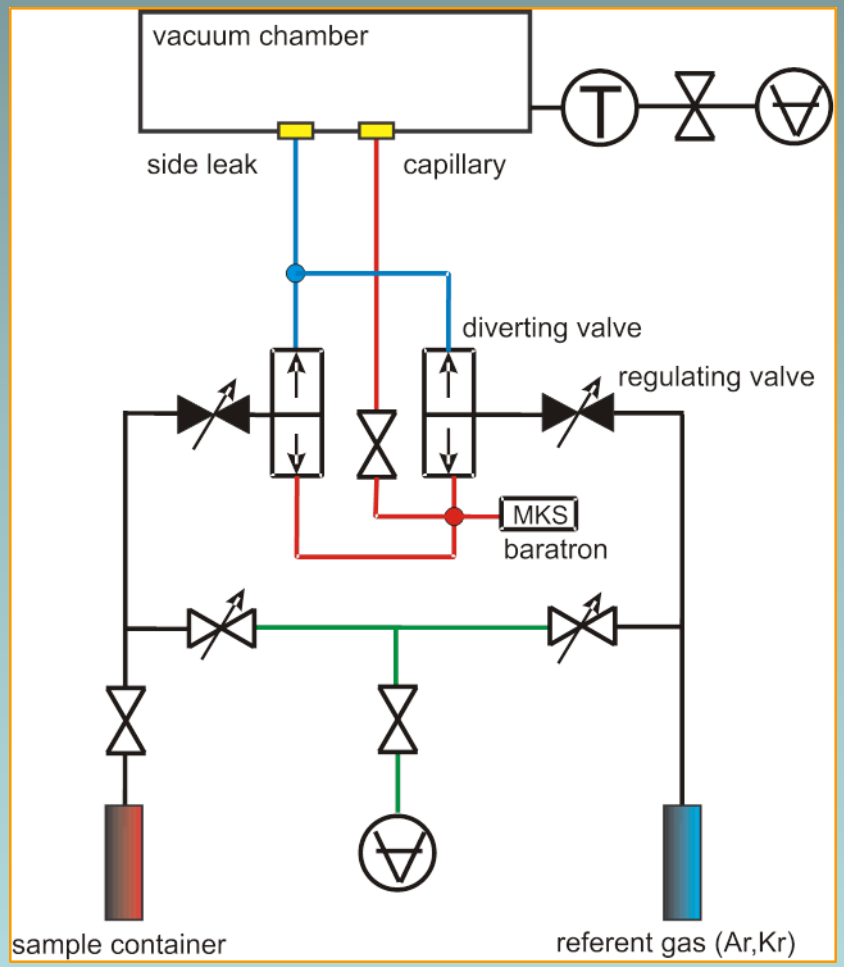
$$DCS_{E_0}(\theta) = \frac{I_{E_0}(\theta)}{\eta(E_0)V_{effE_0}(\theta)}$$

Relative DCSs in the function of incident energy

$$DCS_{\theta}(E_0) = \frac{I_{\theta}(E_0)}{\eta(E_0)V_{eff\theta}(E_0)}$$



Relative flow technique - measuring absolute DCSs



- In the relative flow method, the DCSs for scattering of unknown gas is determined by comparing scattering signals from the standard target with its known differential cross sections, at a given incident electron energy and scattering angle under identical collision geometry conditions

- To obtain the same profiles for both gas beams, the gases must be operated at pressures behind the needle so that their mean free paths are the same.

$$DCSx(E,\theta) = DCSref(E,\theta)\frac{NxFref}{NrefFx}\sqrt{\frac{Mref}{Mx}}$$

$$PV_0 = nkT_0$$

$$\frac{dP}{dt} = \frac{kT_0}{V_0}\frac{dn}{dt} = cF$$

Results

ELASTIC SCATTERING – aneasthetcs – absolute DCSs

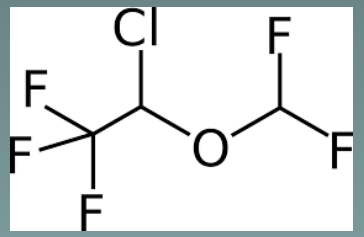
1. *Jelena Vukalović, Jelena B. Maljković, Francisco Blanco, Gustavo García, Branko Predojević, Bratislav P. Marinković,*
"Absolute differential cross-sections for elastic electron scattering from sevoflurane molecule in the energy range from 50-300 eV",Int. J. Molec. Sci. 23(1) 21 (2022)

2. *Jelena B. Maljković, Jelena Vukalović, Zoran D. Pešić, Francisco Blanco, Gustavo García, Bratislav P. Marinković, "Experimental and theoretical study on elastic electron interaction with halothane molecule in the intermediate energy range", Eur. Phys.J. Plus 138, 349 (2023)*

3. *Absolute DCS for elastic electron scattering from Isofluran: submited in PCCP*

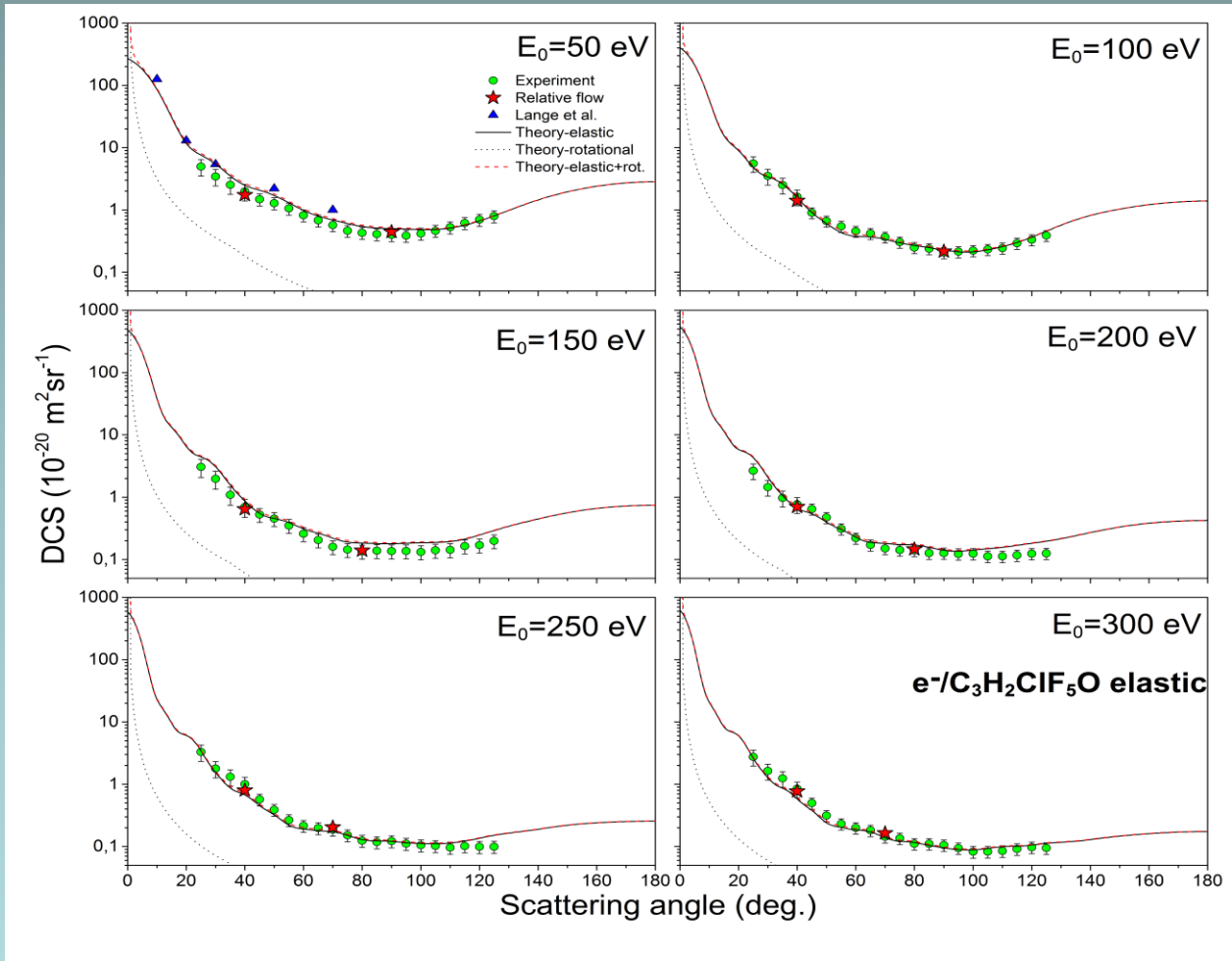
4. *Absolute DCS for elastic electron scattering from Desflurane: preliminary results*

Isoflurane



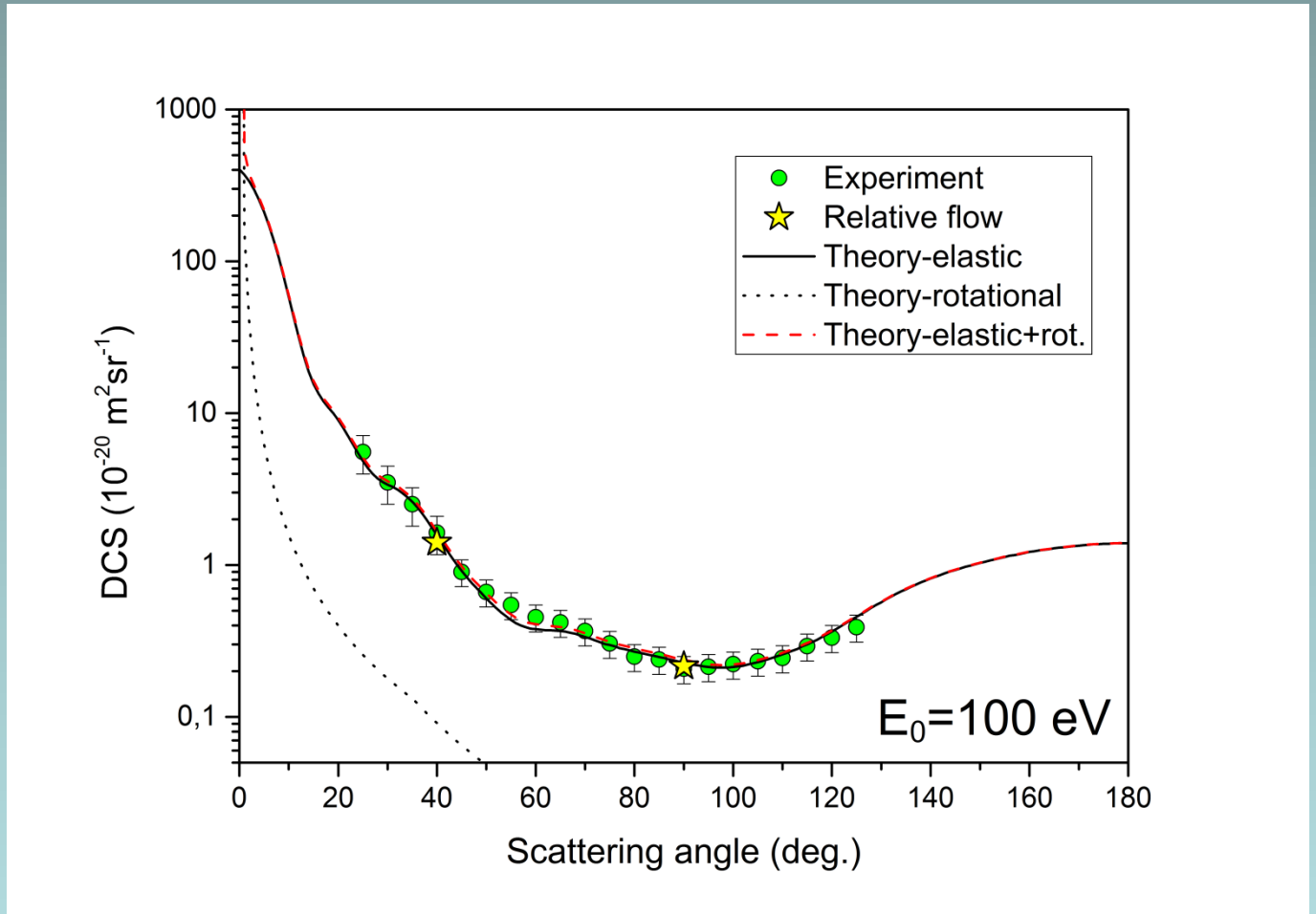
- Isoflurane (2-chloro-2-(difluoromethoxy)-1,1,1-trifluoroethane, $CF_3CHCl\text{-}O\text{-}CHF_2$) has been widely used as an inhalational anesthetic.
- Non-flammable halogenated ether, a clear, colorless liquid with a mild odor. It has a molecular weight of 184.49 g/mol, a boiling point of 48.5 °C, a vapor pressure of 330 mmHg, and an estimated dipole moment of 2.47 D
- Because of its connection to climate change, isoflurane has lately caught the scientific community's attention.
- .It has been shown that the vast majority of anesthetics administered do not undergo metabolization and are consequently discharged unaltered from the patient's body into the lower atmosphere
- The reactivity of the anesthetic compounds with OH radicals determines their fate in the atmosphere, and their atmospheric lifetime can be estimated by measuring the rate coefficient for this reaction.
- atmospheric lifetime of isoflurane is calculated to be between 2 and 5.9 years, long enough to cause some damage
- As a halogenated compound, isoflurane has a high global warming potential (GWP). The isoflurane GWP (for a 100-year time horizon), relative to CO2, was reported by Brown , the WMO , Andersen et al., Langbein et al. and Ryan and Nielsen to be 328, 470, 510, 545, and 571.

ELASTIC SCATTERING – *absolute DCSs isoflurane(as a function of scattering angle)*

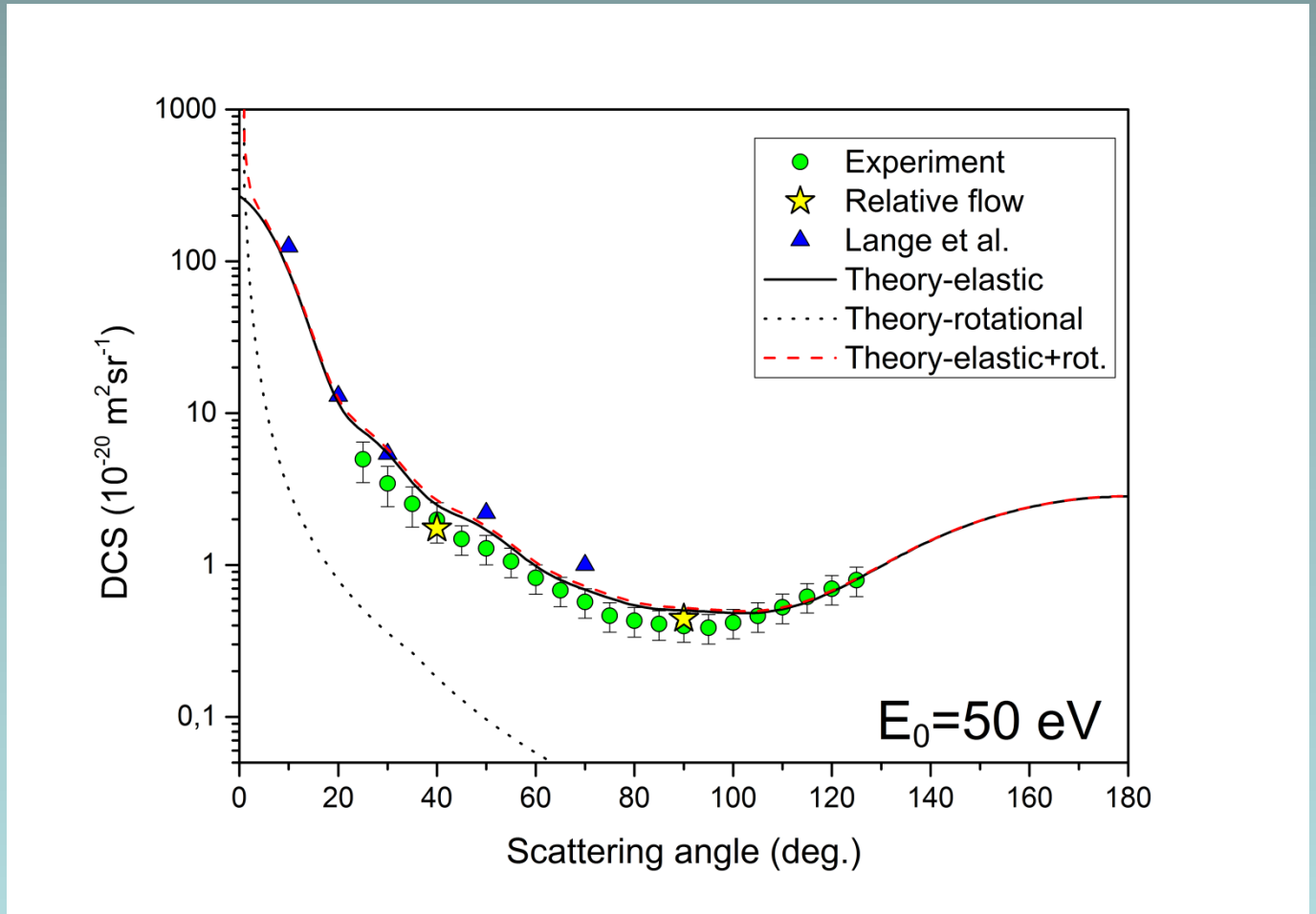


ELASTIC SCATTERING – *absolute DCSs*

isoflurane, 100eV(as a function of scattering angle)



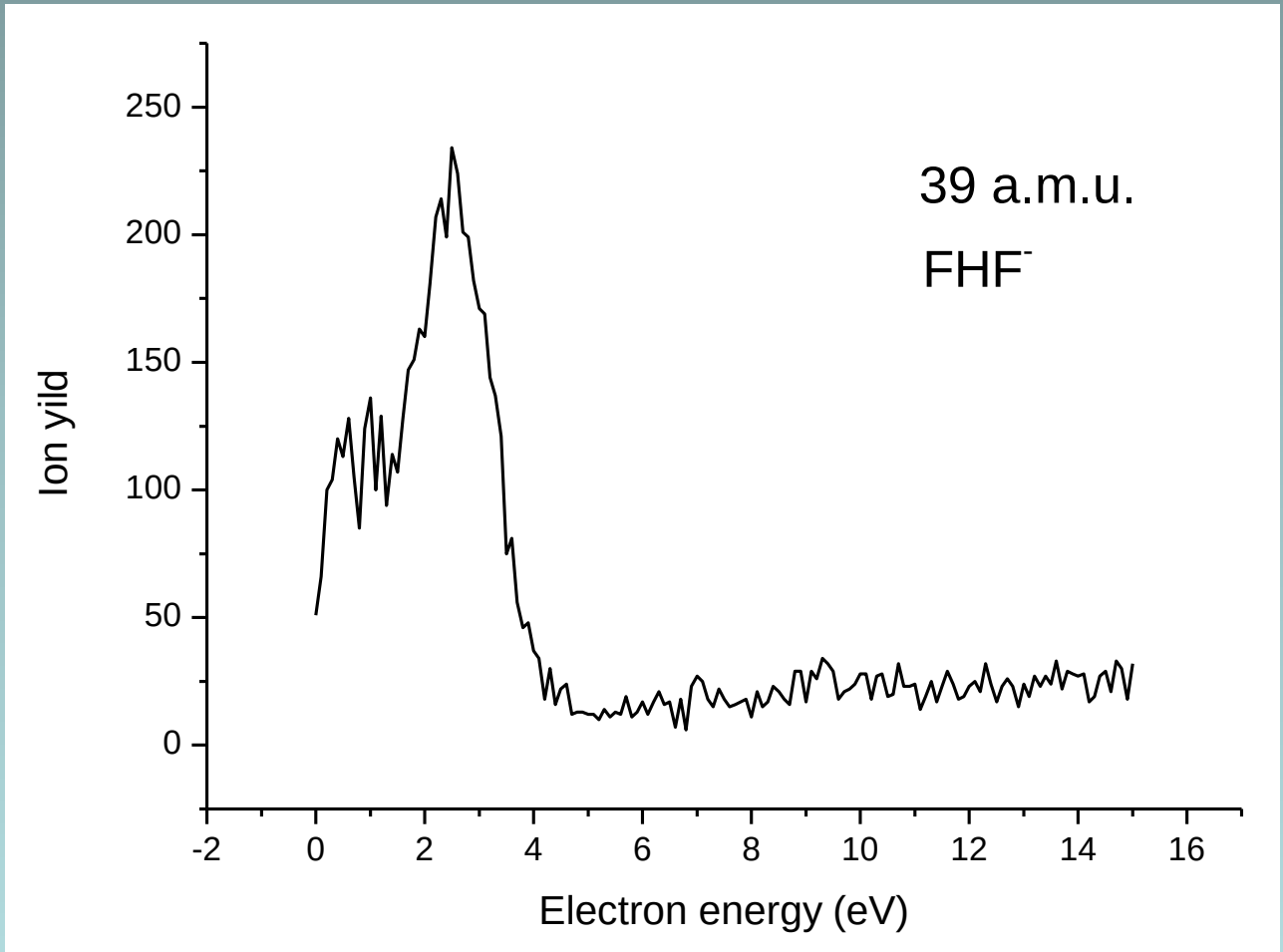
ELASTIC SCATTERING – *absolute DCSs isoflurane, 50eV(as a function of scattering angle)*



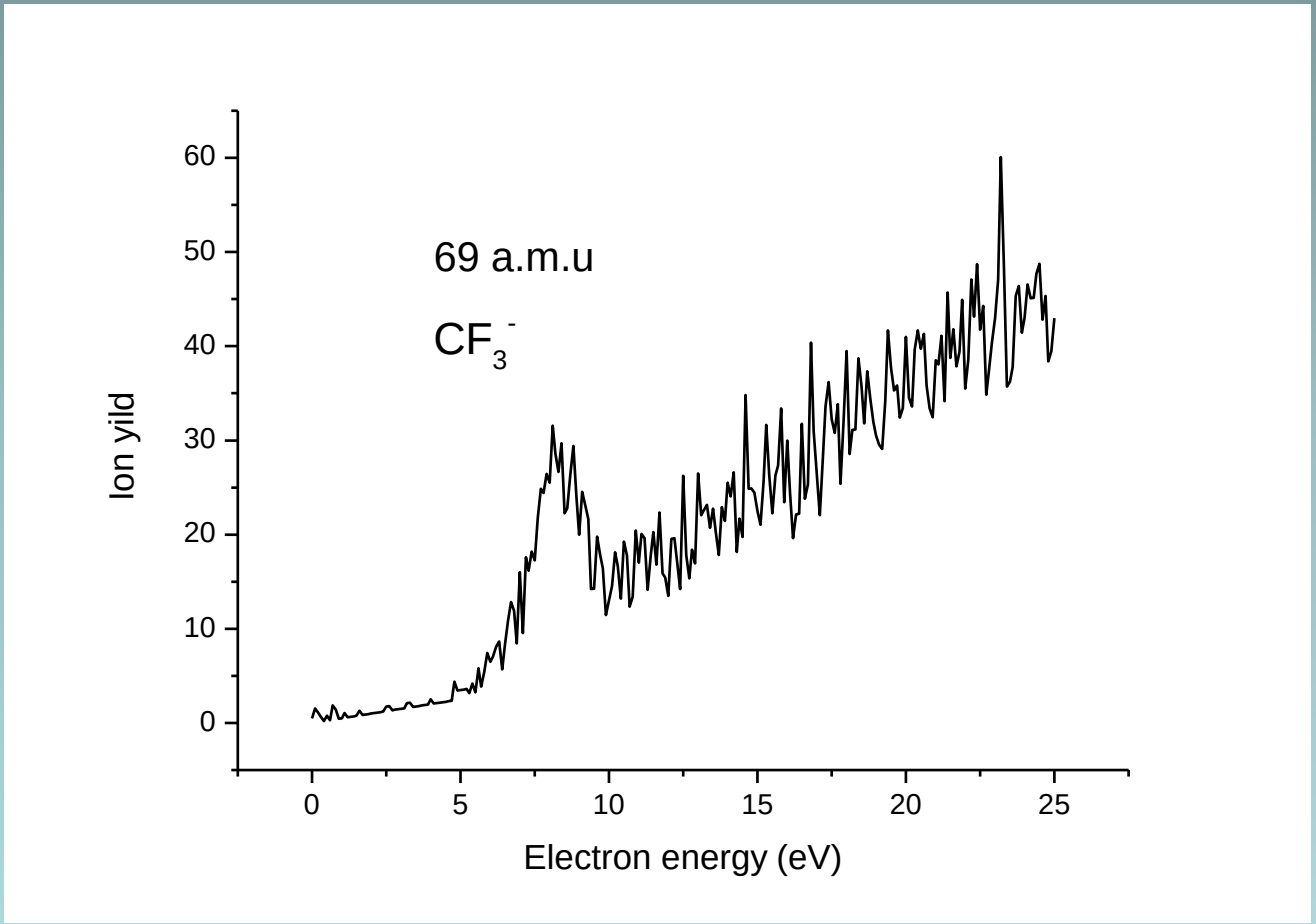
DEA

- We studied DEA to gas phase target by means of a crossed electron-molecular beam technique.
- The measurements of the yield of negative fragments at defined electron energies were measured (mass scans) and the intensity of the generated anions were measured as a function of incident electron energy.
- We have measured halogenated aneasthetic isofluran ($C_3H_2ClF_5O$) which showed a rich fragmentation.
- Dissociative electron attachment processes were investigated utilizing the crossed beam apparatus settled at University of Natural Science and Humanities in Siedlce, Poland.
- Incident electron beam orthogonally intersects with molecular beam resulting in the formation of fragmentanions.. The calibration of the energy scale is achieved by measuring SF_6signal, with intense resonance near 0 eV. Base pressure was in the range of ~10^{-8}mbars.
- We assume that lower energy peaks are overlapping resonances in the energy range around 0-11eV which arise from DEA processes and above 15eV constant increase of the yield is due do dipolar dissociation.

Energy scan on the mass that due to FHF- yild, electron energy 0-15eV

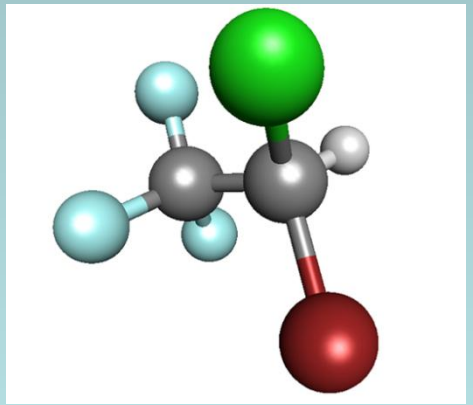


Energy scan on the mass that due to CF_3- yild, electron energy 0-25eV

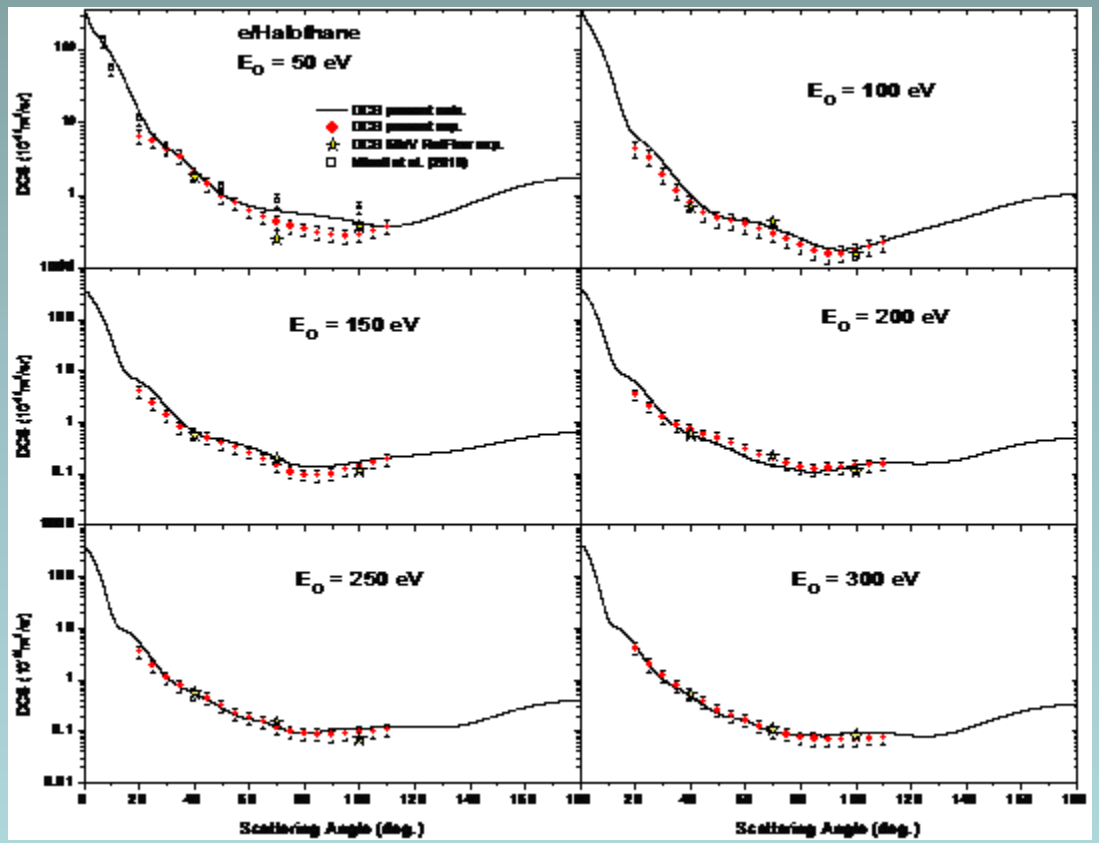


Halothane

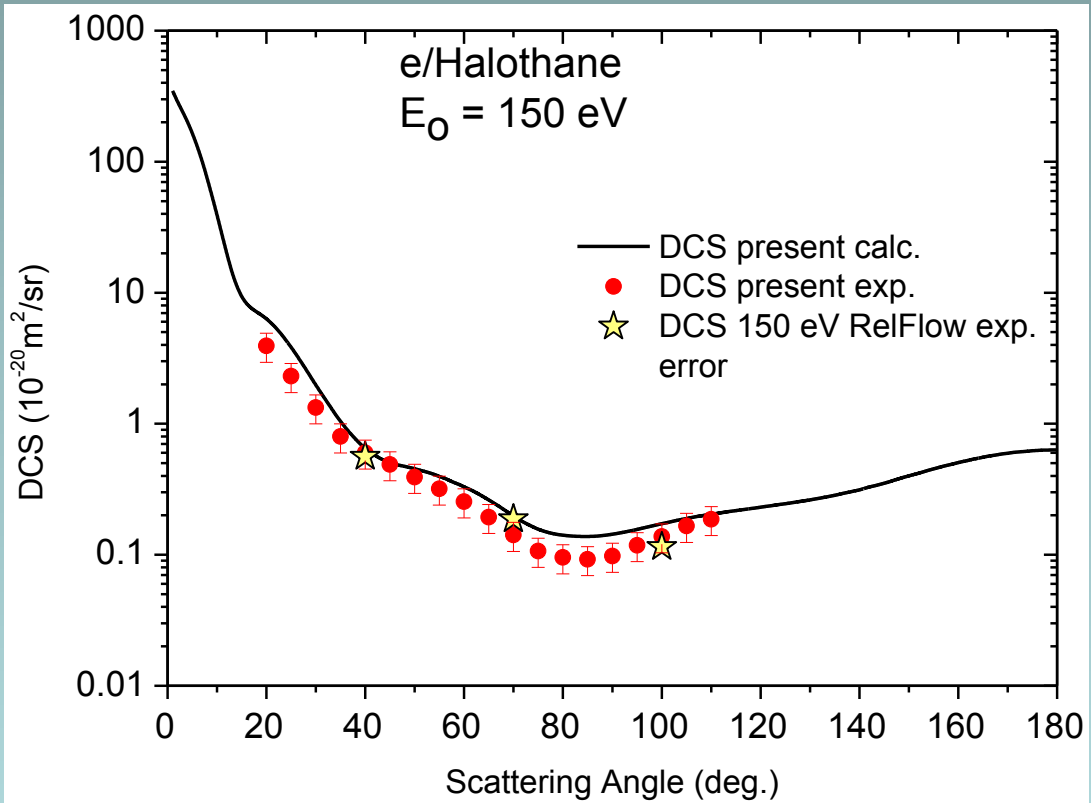
- Halothane is the common name for 2-bromo-2-chloro-1,1,1-trifluoroethane ($CF_3CHBrCl$), a multihalogenated derivate of ethane. It is a clear, colorless, highly volatile liquid, with a sweet chloroform-like odor. Its boiling point is 50.2 °C, molar mass 197.379 g/mol, vapor pressure 243 mmHg , and dipole moment 1.41 D .
- Study by Langbein et al. (OH reactivity + UV absorption spectra) showed that the tropospheric lifetime of halothane is about 7 years. This means that emitted halothane gas can reach the stratosphere in a considerable amount (more exactly 13,2 % according to Langbein et al.). The ozone depletion potential (ODP) of halothane is estimated 1.56 , relative to one of CFC-11 (freon-11), and is the highest among all anesthetics. This high ODP is due to its bromine content.
- All of the above indicates that the influence of the halothane on global warming and ozone destruction should not be ignored. Therefore, the significance of researching the electron interactions with the mentioned molecule is clear.



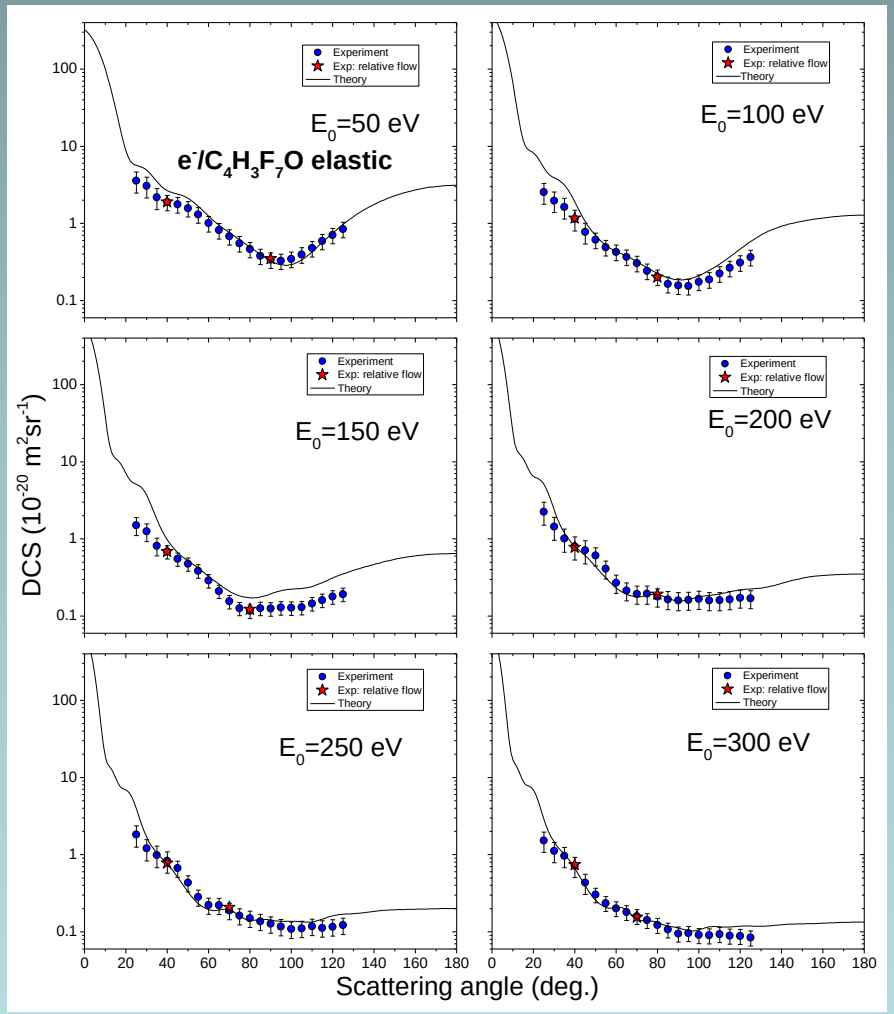
ELASTIC SCATTERING – *absolute DCSs*
Halothane, from 50 - 300 eV(as a function of scattering angle)



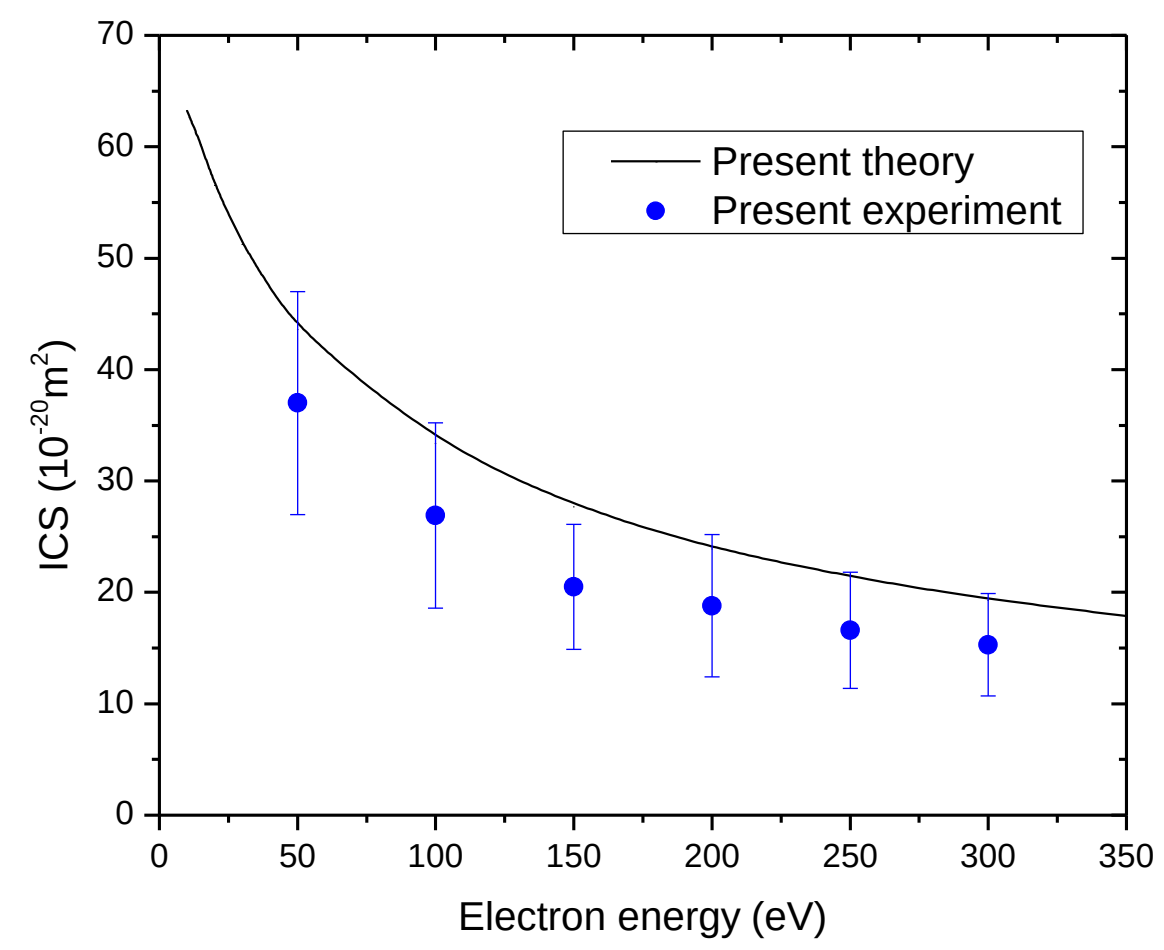
ELASTIC SCATTERING – *absolute DCSs*
Halothane, 150eV(as a function of scattering angle)



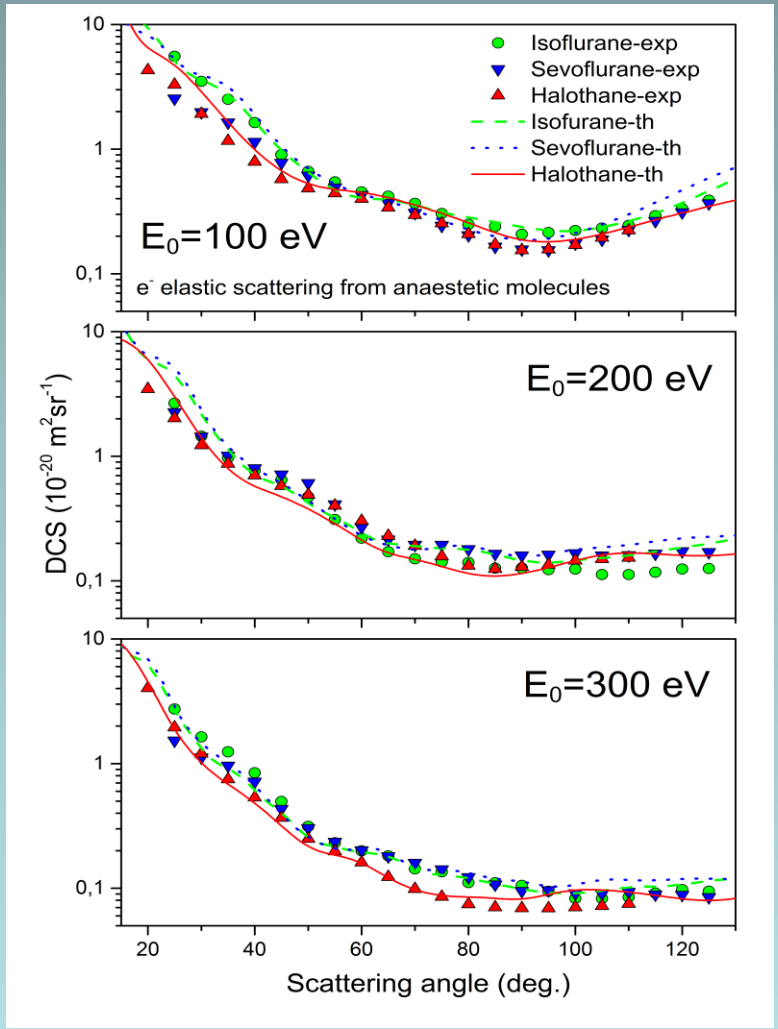
ELASTIC SCATTERING – *absolute DCSs*
Sevofluran, 50 - 300 eV(as a function of scattering angle)



ELASTIC SCATTERING – Sevoflurane *Integral cross sections*

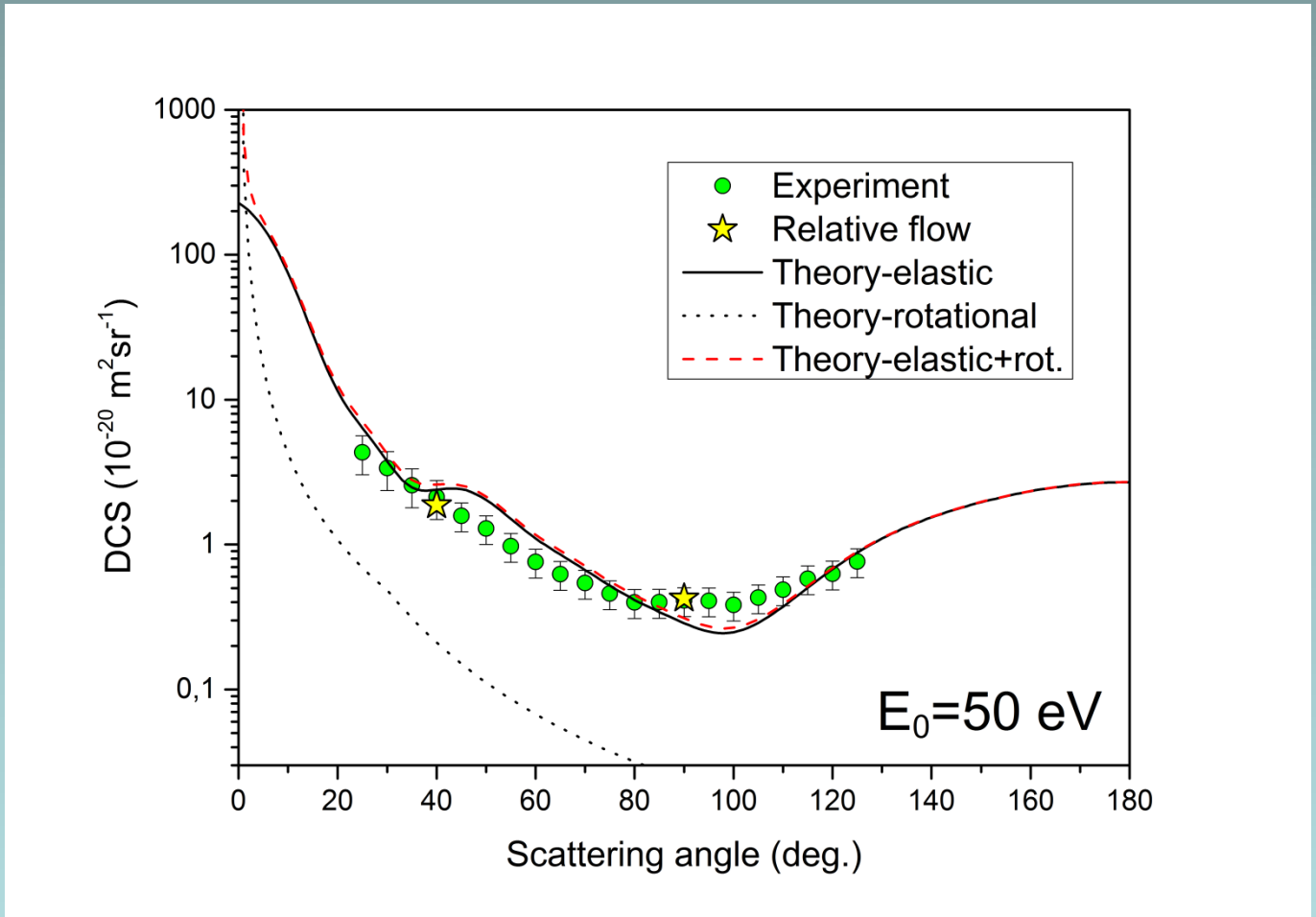


Comparison of absolute DCSs: isoflurane, sevoflurane and haloten at 100 eV 200eV and 300 eV



ELASTIC SCATTERING – *absolute DCSs*

Desfluran, 50 eV(as a function of scattering angle, preliminary results)



ELASTIC SCATTERING – biomolecules – *absolute DCSs*

Triethyl phosphate: Jelena B. Maljković, Jelena Vuković, Károly Tökési, Branko Predojević, and Bratislav P. Marinković, **Eur. Phys. J.D 73, 27 (2019)**

Furan: J. B. Maljković, F. Blanco, R. Čurik, G. García, B. P. Marinković, and A. R. Milosavljević, J. Phys. Chem. 137 064312 (2012).

Formamide: J. B. Maljković, F. Blanco, G. García, B. P. Marinković, and A. R. Milosavljević, Nucl. Instrum. Meth. B.
279, 124 (2012)

.**N-methyl formamide:** *J.* B. Maljković, F. Blanco, G. García, B. P. Marinković, and A. R. Milosavljević, Phys. Rev. A 85, 042723 (2012).

Pyrimidine: J. B. Maljković, A. R. Milosavljević, F. Blanco, D. Šević, G. García and B. P. Marinković, *Phys. Rev. A* **79** 052706 (2009)

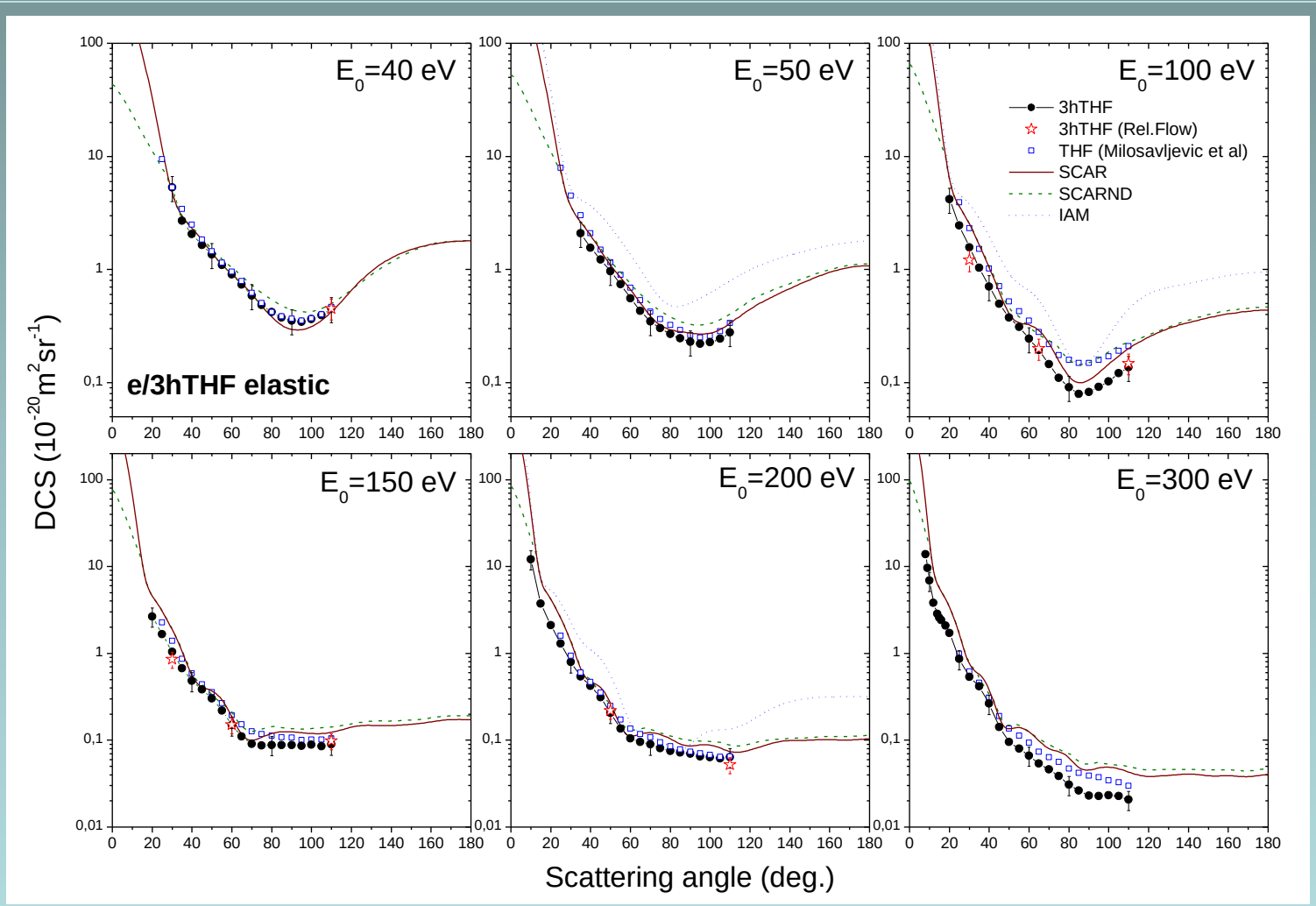
3-hydroxytetrahydrofuran: A. R. Milosavljevic, F Blanco, J B Maljkovic, D Sevic, G García and B P Marinkovic, *New Journal of Physics* **10** 103005 (2008)

Tetrahydrofuran: M. Dampc, A. R. Milosavljević, I. Linert, B. P. Marinković, and M. Zubek, *Phys. Rev. A* **75**, 042710 (2007)

Tetrahydrofurfuryl alcohol: A. R. Milosavljević, F. Blanco, D. Ševic, G. Garcia and B.P. Marinković, *Eur. Phys. J. D* **40**, 107-114 (2006)

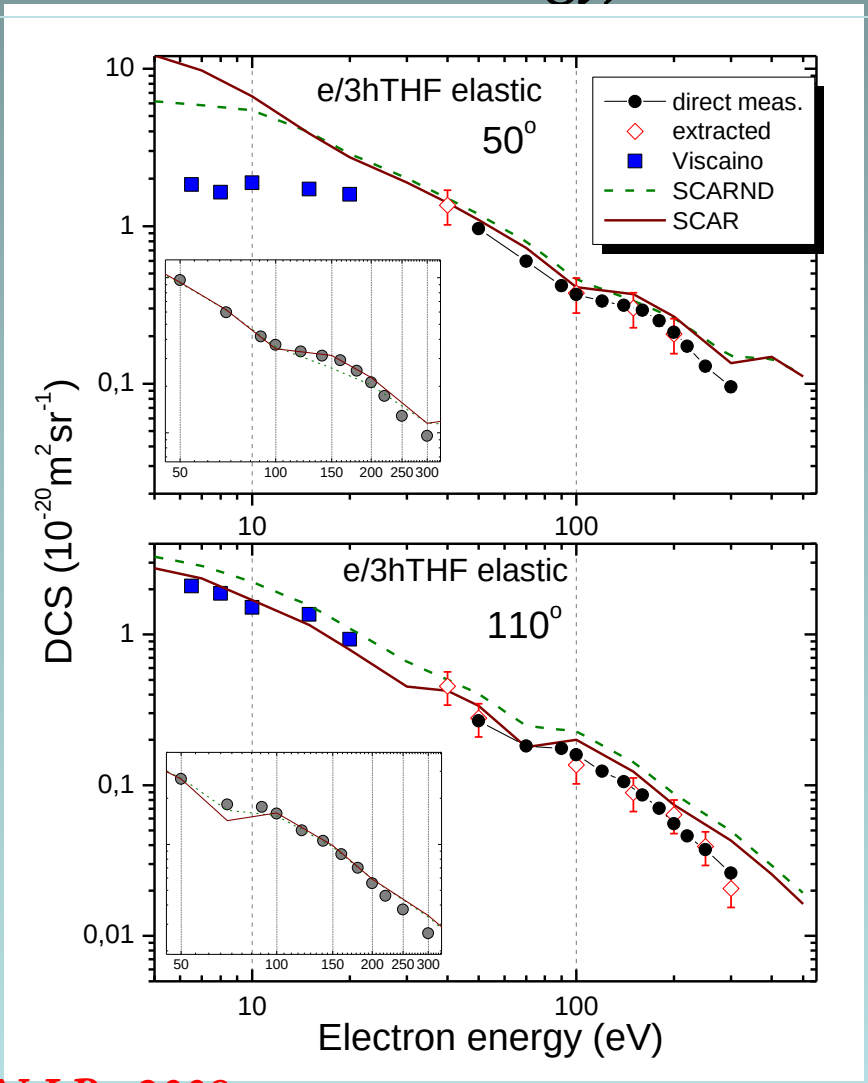
Tetrahydrofuran: A. R. Milosavljević, A. Giuliani, D. Ševic, M.J. Hubin-Franskin and B.P. Marinković, *Eur. Phys. J. D* **35**, 411-416 (2005)

ELASTIC SCATTERING – *absolute DCSs*
3-hydroxytetrahydrofuran(as a function of scattering angle)



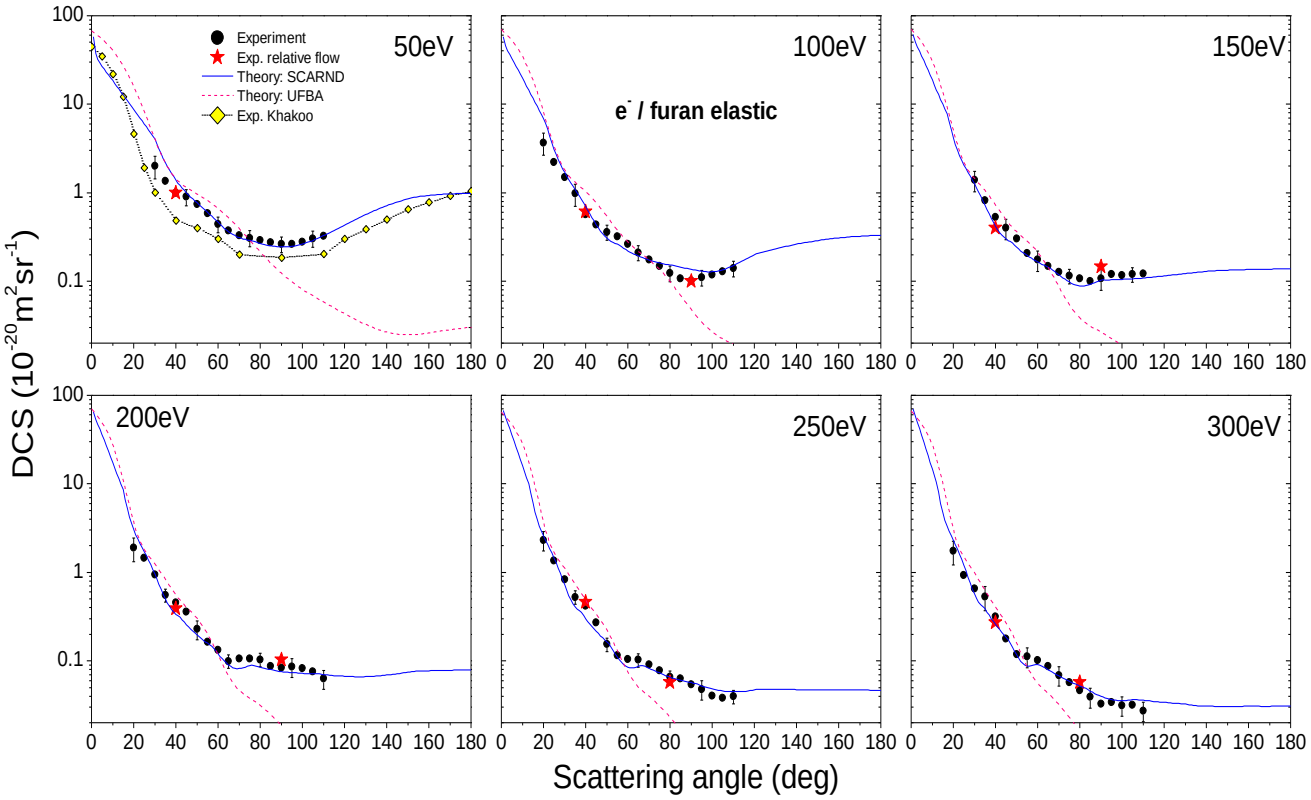
Milosavljević et al, N.J.P., 2009

ELASTIC SCATTERING – *absolute DCSs*
3-hydroxytetrahydrofuran (as a function of incident electron energy)



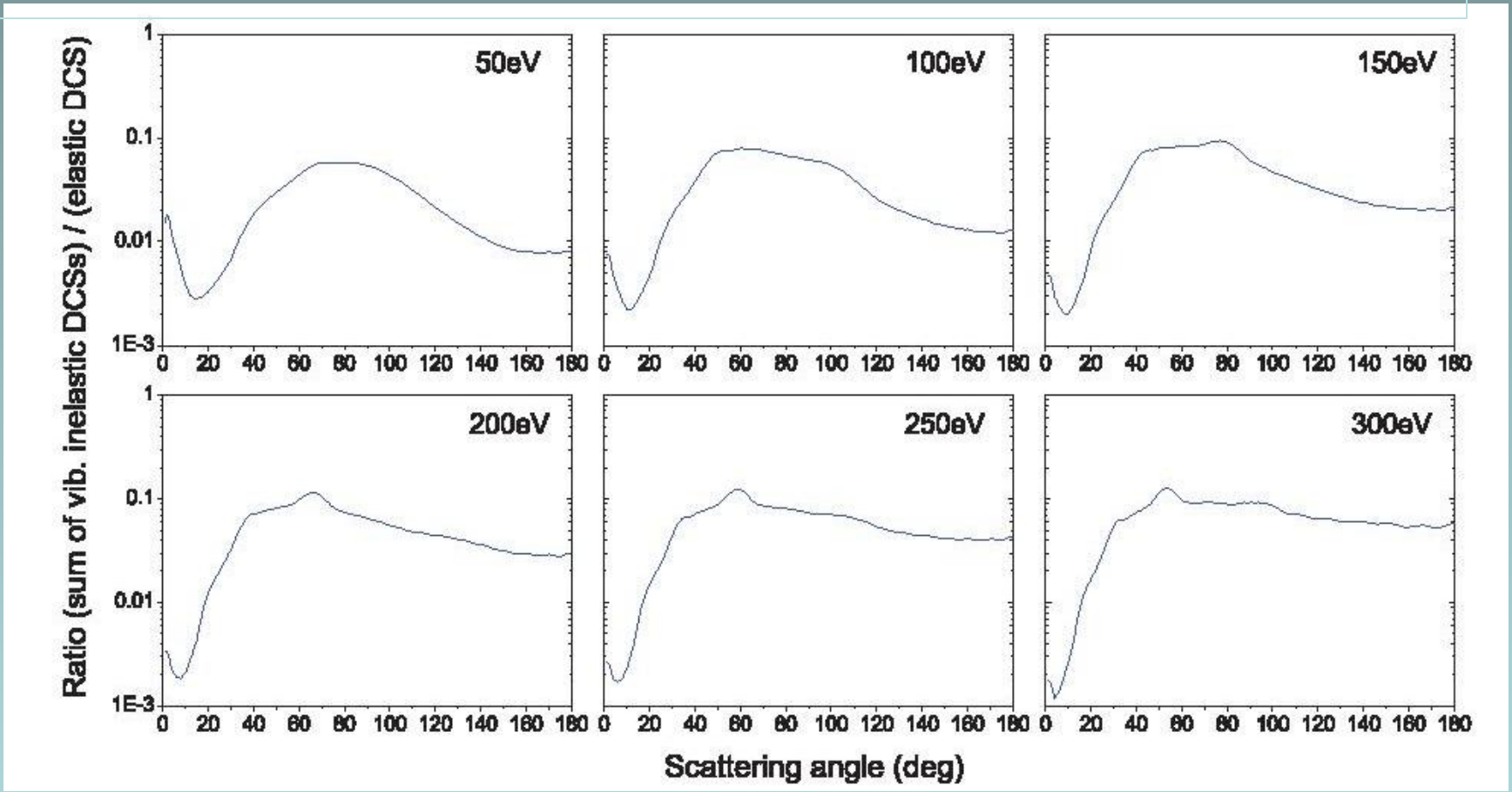
Milosavljević et al, N.J.P., 2009

ELASTIC SCATTERING – *absolute DCSs*
furan (as a function of scattering angle)



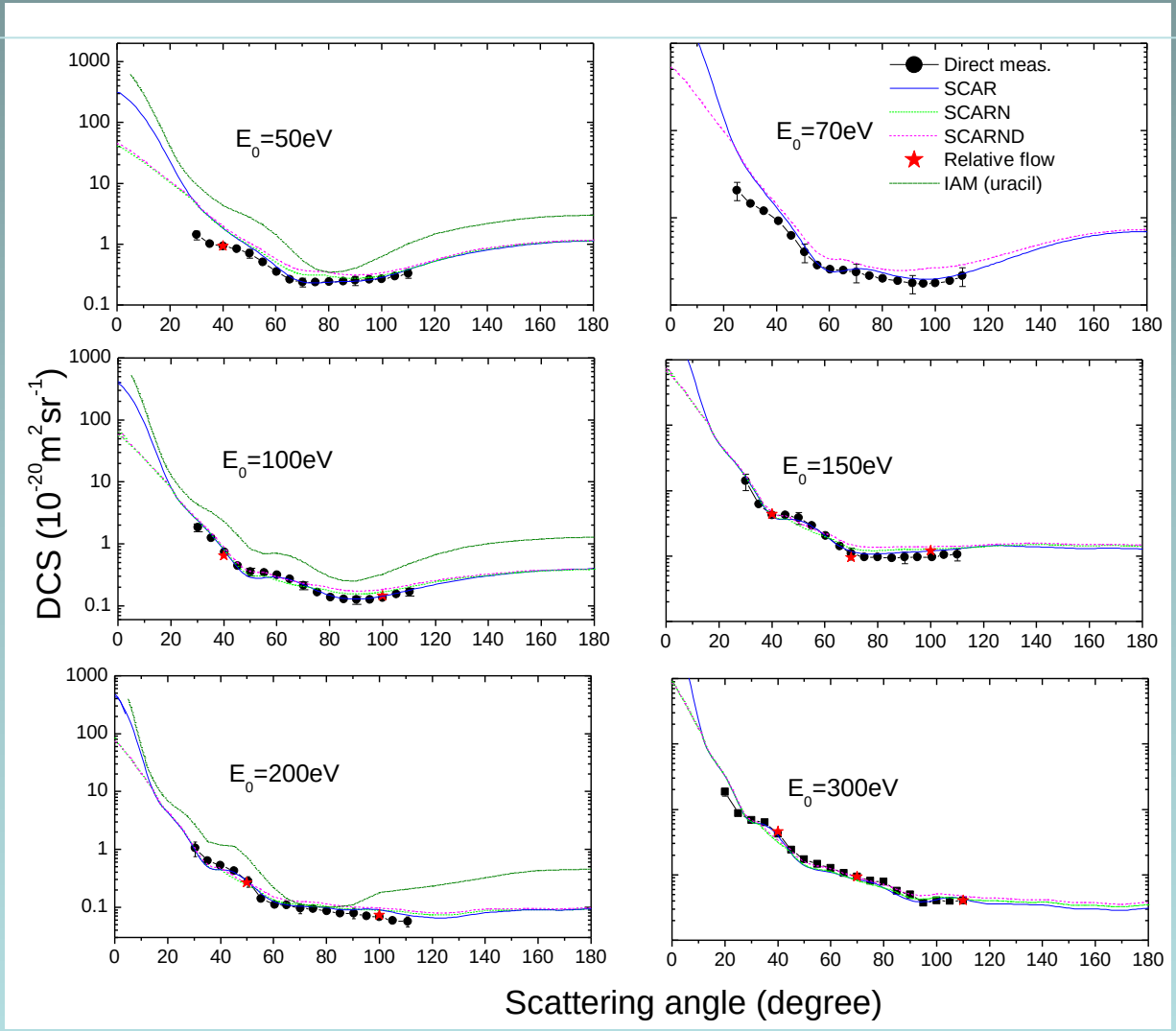
Maljković et al, J.Phys.Chem., 2012

RATIO VIBRATIONAL / ELASTIC CROSS SECTIONS (furan)



Maljković et al, J.Phys.Chem., 2012

ELASTIC SCATTERING – *absolute DCSs*
Pyrimidine(as a function of scattering angle)



Maljković et al, PRA, 2009

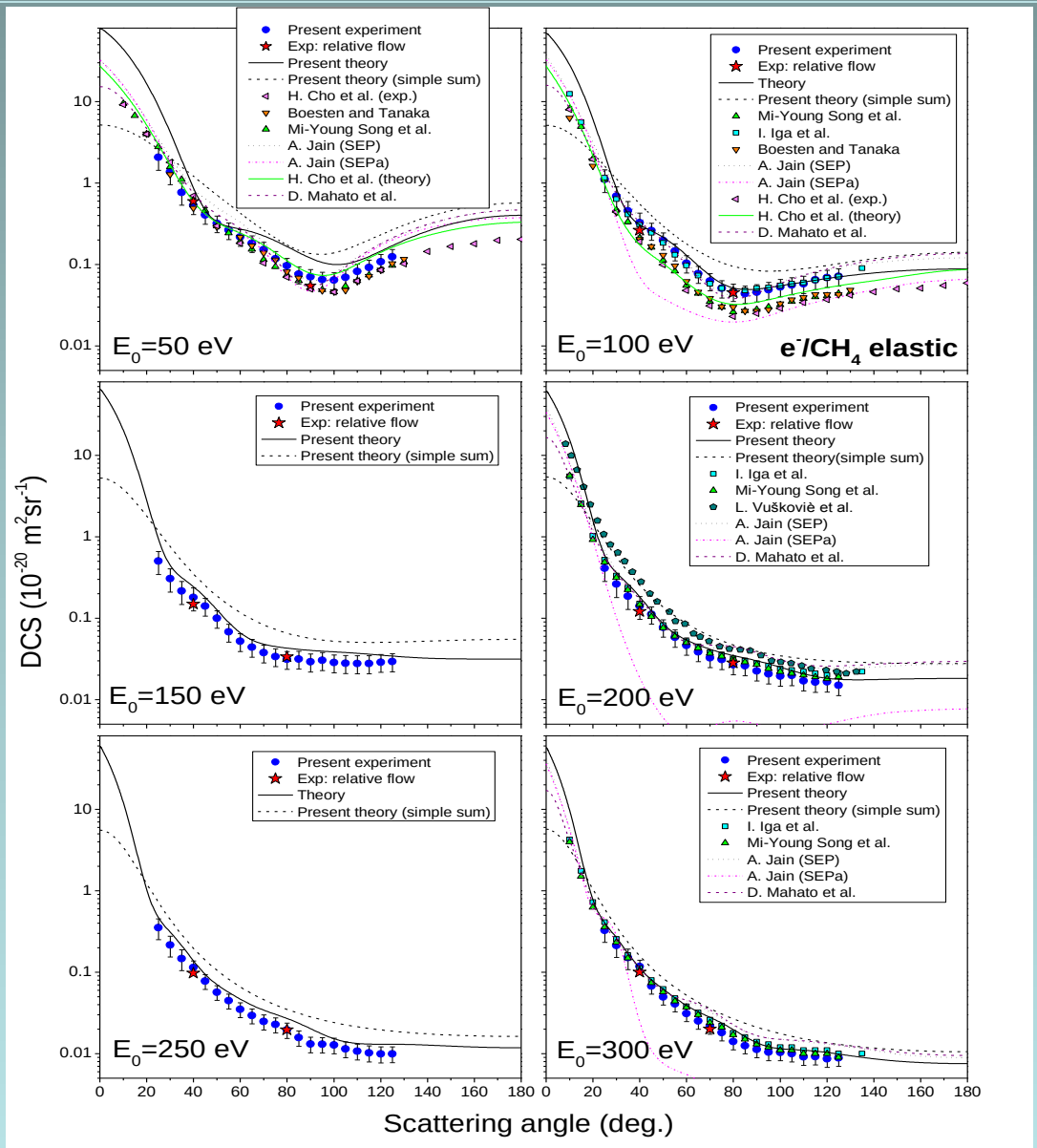
Why methane

- Methane (CH_4) is the simplest hydrocarbon molecule and has attracted significant interest as a target for energy electron collision studies.
- Major component of the atmosphere of the outer planets (Jupiter, Saturn, Uranus, Neptune) and their satellites
- Present in plasma technologies, e.g. plasma synthesis of diamonds
- Methane is one of the most prevalent long-lived greenhouse gases (together with carbon dioxide and nitrous oxide). Greenhouse effect caused by methane is 8 times higher than of CO_2. Emmision of methane in atmosphere is about 40% natural and 60% antropogenic causes.
- It has many technological and atmospheric applications as well as a fundamental importance as one of the testing grounds for the collision theories.
- Because methane grow rate is increased in past decades it become again important to investigate this gas and it is important to understand its interaction mechanism with other molecules, atoms and particles, including electrons.

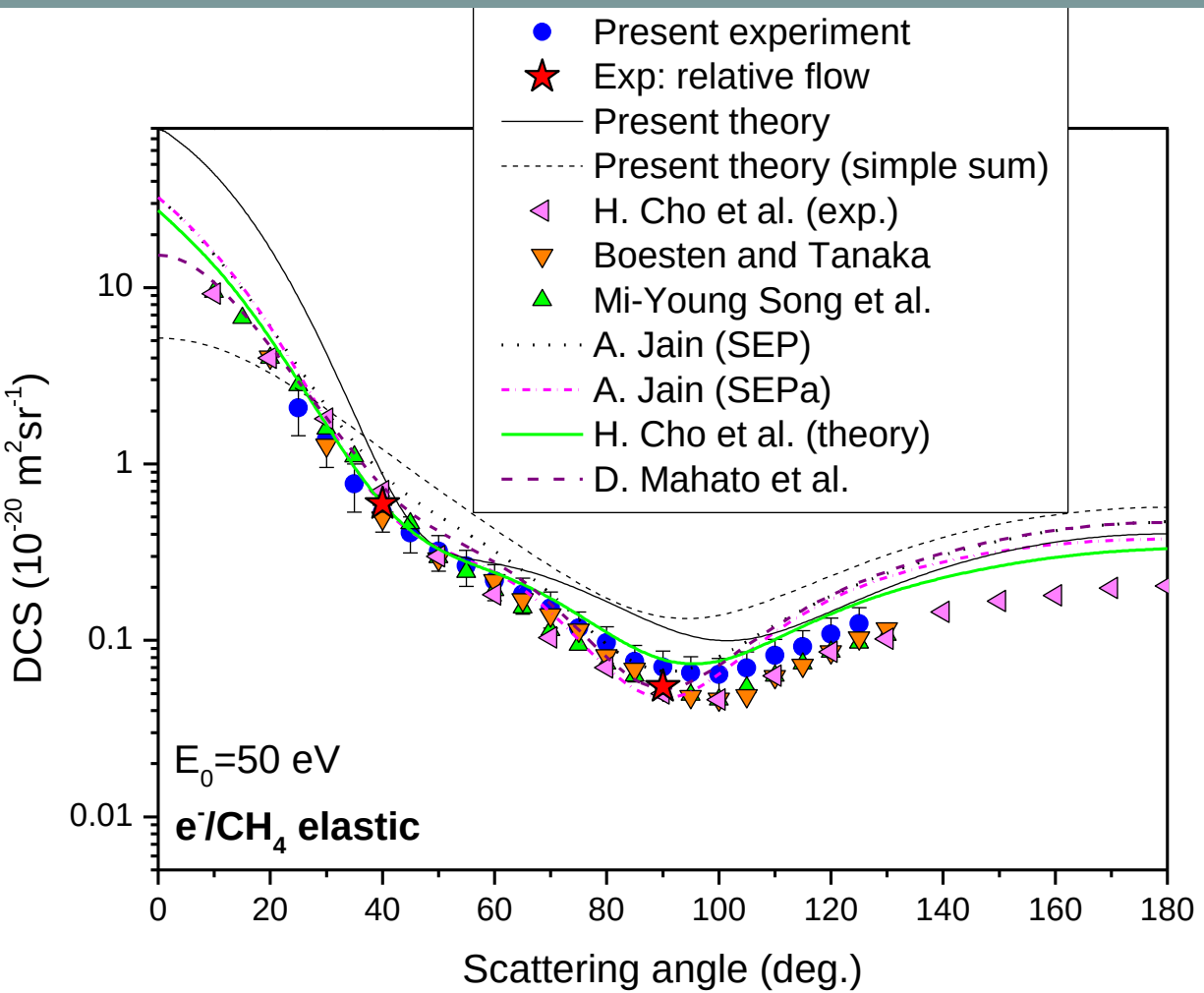
List of experimental and theoretical work on DCS for elastic scattering of electrons from methane molecule, covering energy range from 50 to 300 eV.

Authors	Experiment type with normalization method/ theoretical approach	Energy range (eV)	Angular range (°)
Boesten and Tanaka [11]	Crossed beams, simultaneous measurements of DCS of He	1,5-100	10-130
Vušković and Trajmar [12]	Crossed beams, normalized to other authors results	20-200	8-130
Cho et al. [15]	Crossed beams, relative flow (He)/ Schwinger variational method	5-100	10-180
Sakae et al. [16]	Crossed beams, relative flow (He)	75-700	5-135
Iga et al. [17]	Crossed beams, relative flow (Ne)/ Schwinger variational method	100-500/ 1-500	10-135
Jain [18]	Spherical optical complex potential model	0,1-500	0-180
D. Mahato et al. [18a]	Gaussian wave functions	10-500	0-180
Song et al. [19]	Averaging other authors data	1-500	10-140

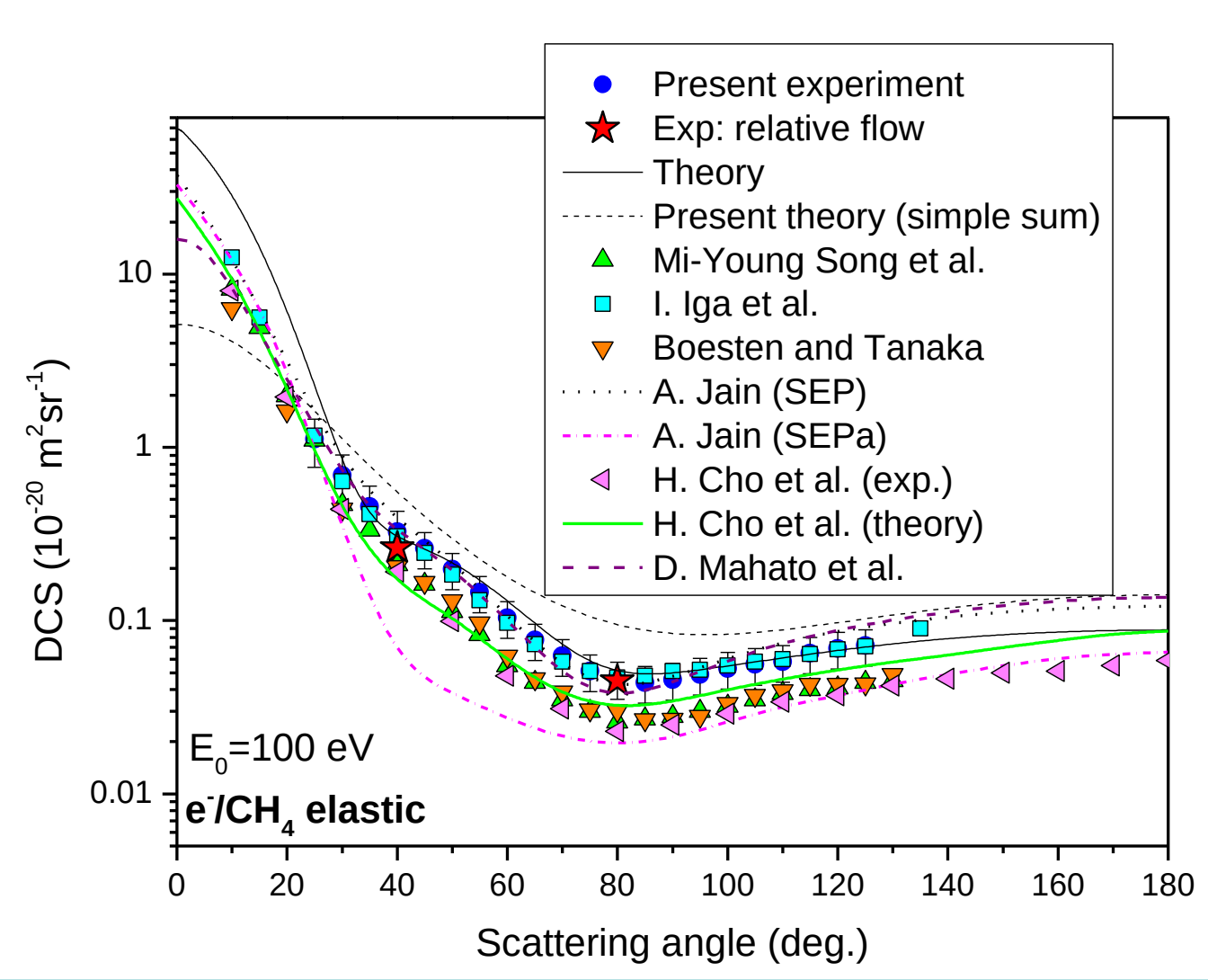
ELASTIC SCATTERING – *absolute DCSs*
Methane (as a function of scattering angle)



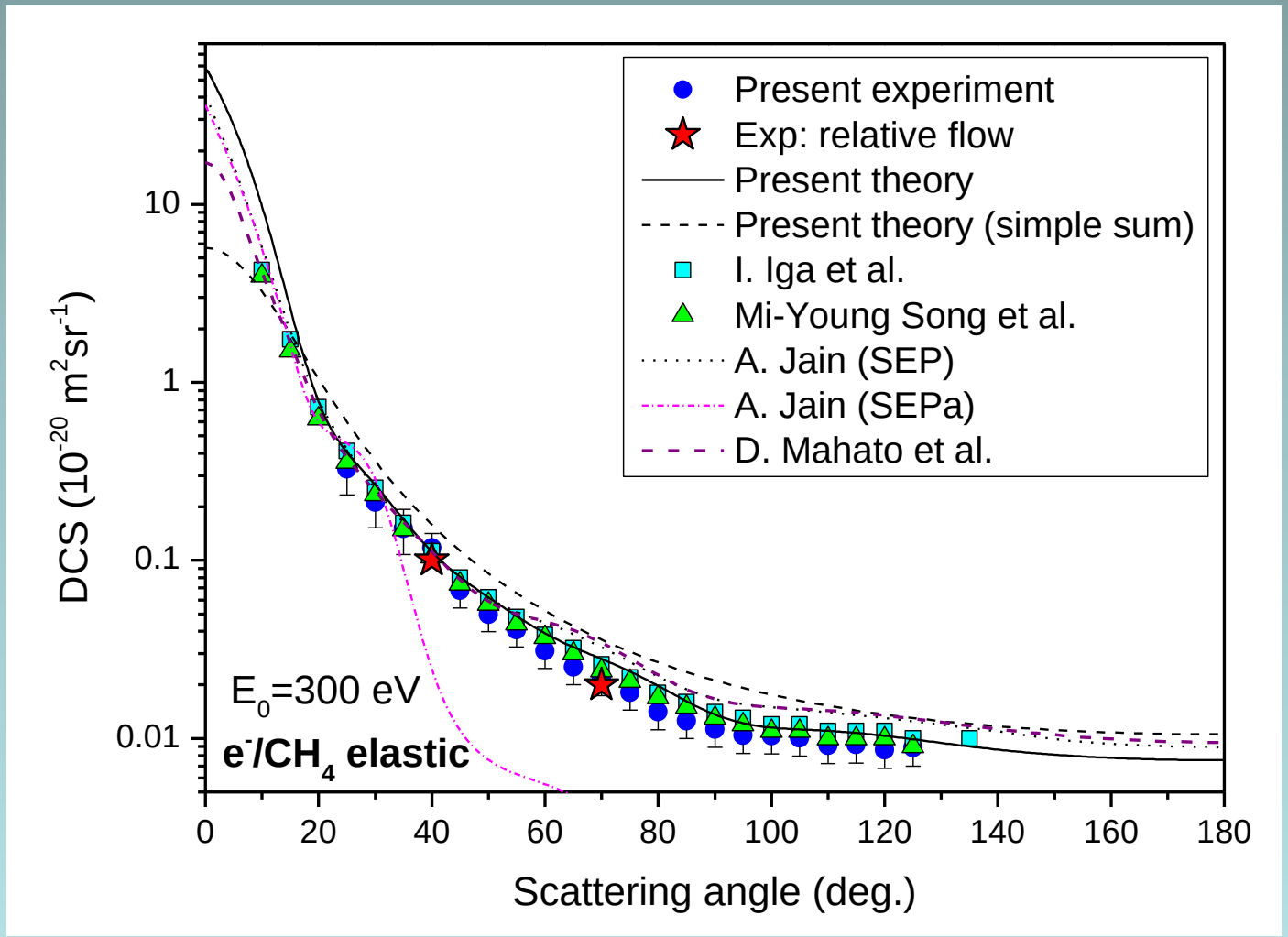
ELASTIC SCATTERING – *absolute DCSs*
Methane, 50eV(as a function of scattering angle)



ELASTIC SCATTERING – *absolute DCSs*
Methane, 100eV(as a function of scattering angle)

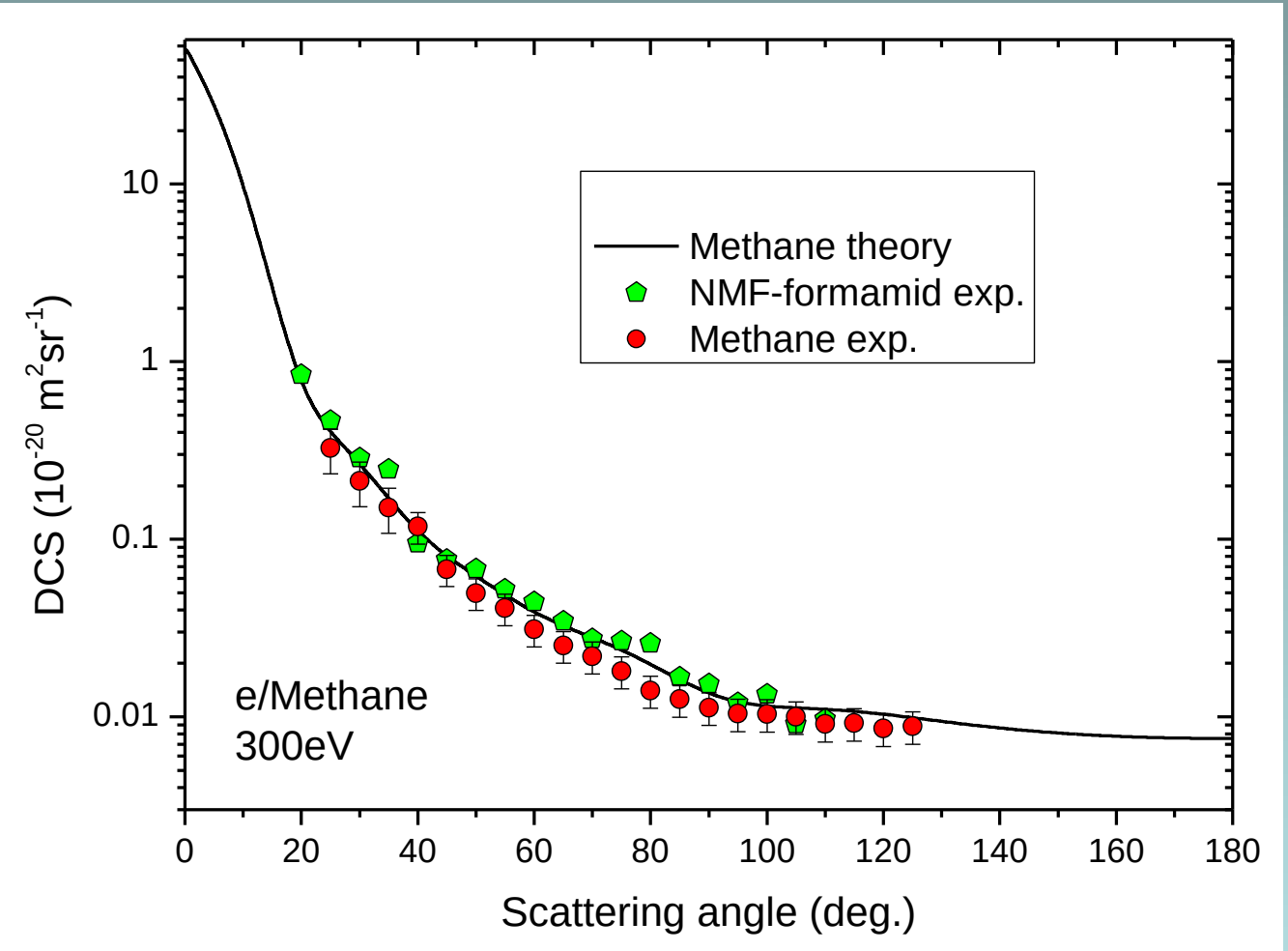


ELASTIC SCATTERING – *absolute DCSs*
Methane, 300eV(as a function of scattering angle)



ELASTIC SCATTERING – *absolute DCSs*

comparison of Methane and NMF-formamide , 300eV



Conclusion

- **Measurements are done by cross beam method, on the electron spectrometer UGRA, for incident energies from 50-300eV.**
- **Absolute differential cross sections for Ar, biomocules, anaesthetic and methane are shown**
- **Calculations are in good agreement with experiment on the absolute scale.**
- **This results contribute to fundamental understanding of electron-molecule (in the gas phase) interactions in the middle energy range.**

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