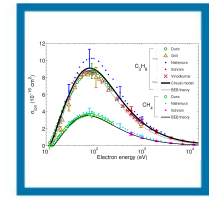
Physikalisch-Technische Bundesanstalt
Braunschweig and Berlin
National Metrology Institute

Potential implementation into Geant4-DNA: **nitrogen, propane** and **DNA cross sections** for electrons and light ions

H. Nettelbeck[1], C. Villagrasa[2], M. Bug[1], S. Meylan[2]

[1]Physikalisch-Technische Bundesanstalt (PTB), Germany
[2]Institut de Radioprotection et de Sûreté Nucléaire (IRSN), France



IRSN INSTITUT DE RADIOPROTECTION ET DE SÛRETÉ NUCLÉAIRE

Motivation

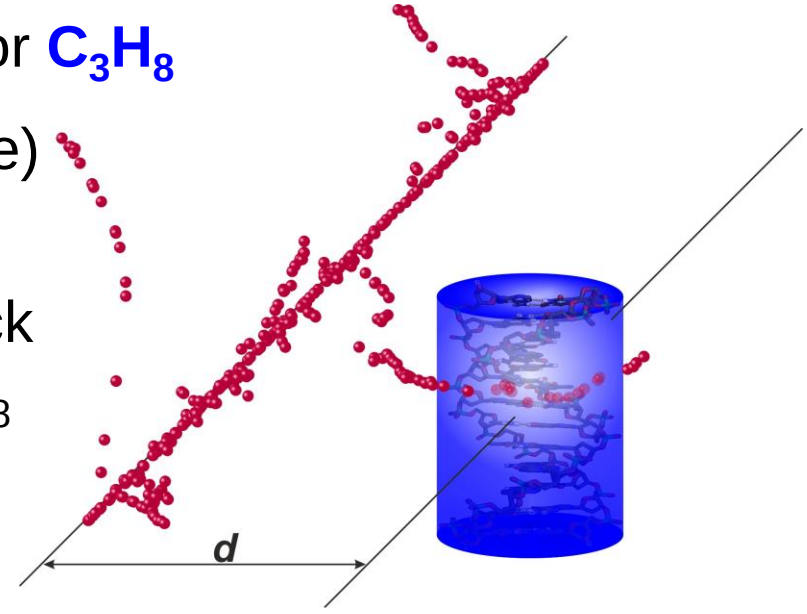
Microdosimetry:

- Tissue-equivalent (TE) proportional counters
- Usually operated in propane-based TE gas
  N_2 , CO_2 , **C_3H_8**

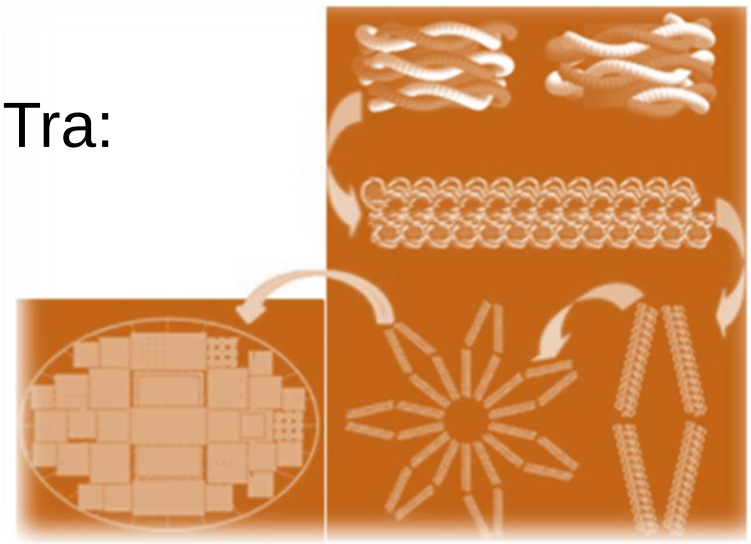
Rossi TE Proportional Counter

Nanodosimetry:

- Nanodosimeters operate with **N_2** or **C_3H_8**
- Ionisation cluster size (measurable)
  ⇨ related to DNA damage
- *PTra* code (PTB) – capable of track structure simulations in N_2 or C_3H_8



Motivation



Advantages of Geant4-DNA over PTra:

- More sophisticated geometry models
- Simulate chemistry processes (radical production and tracking)

Geant4-DNA 10.3 physics models only for *liquid water*

Cross sections of *DNA* constituents (i.e. bases) for e-s and ions

→ Recently implemented in Geant4-DNA 10.4beta
→ Collaboration between IRSN and PTB

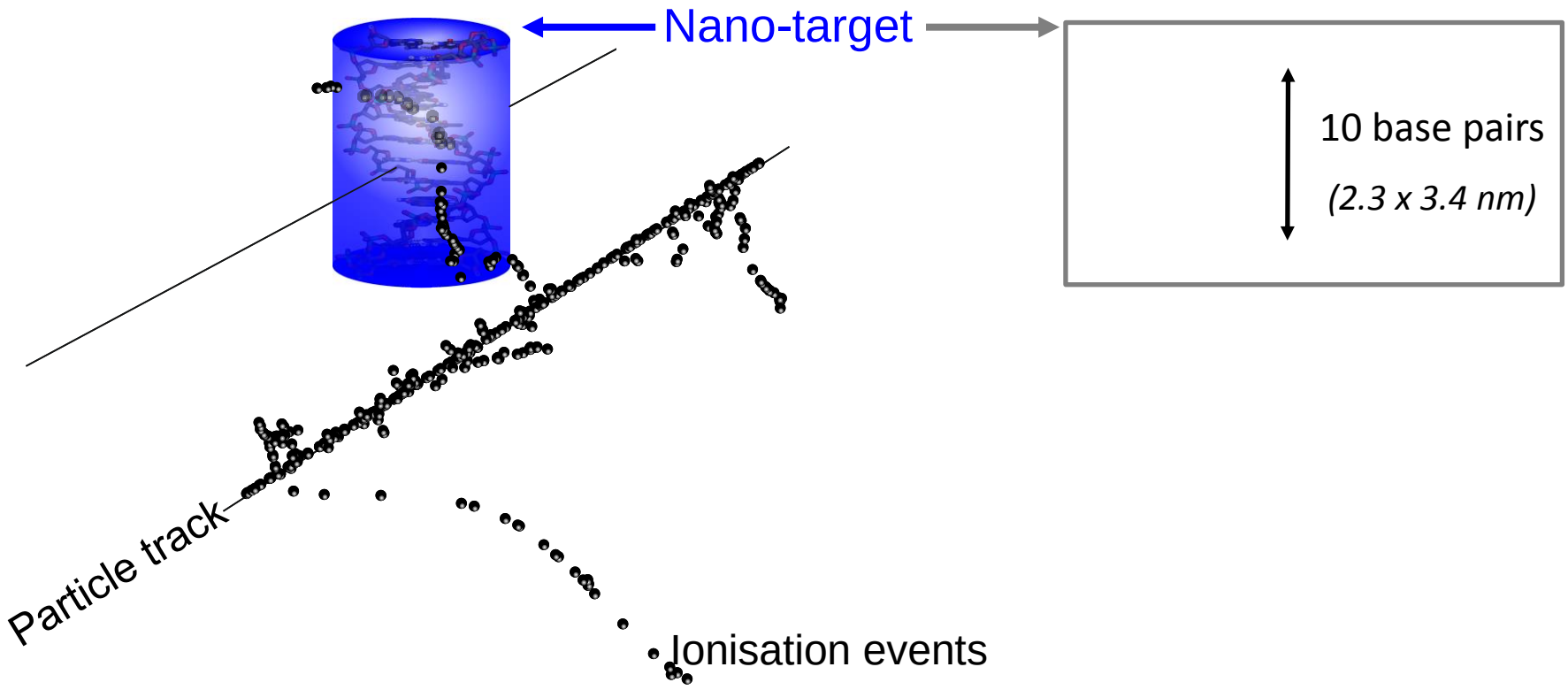
Further development: Include CS of *propane* and *nitrogen* for electrons and ions (micro- and nanodosimetry)

Nanodosimetry

Assumes initial DNA damage due to number of ionisations

→ Directly within short segments of DNA or its vicinity

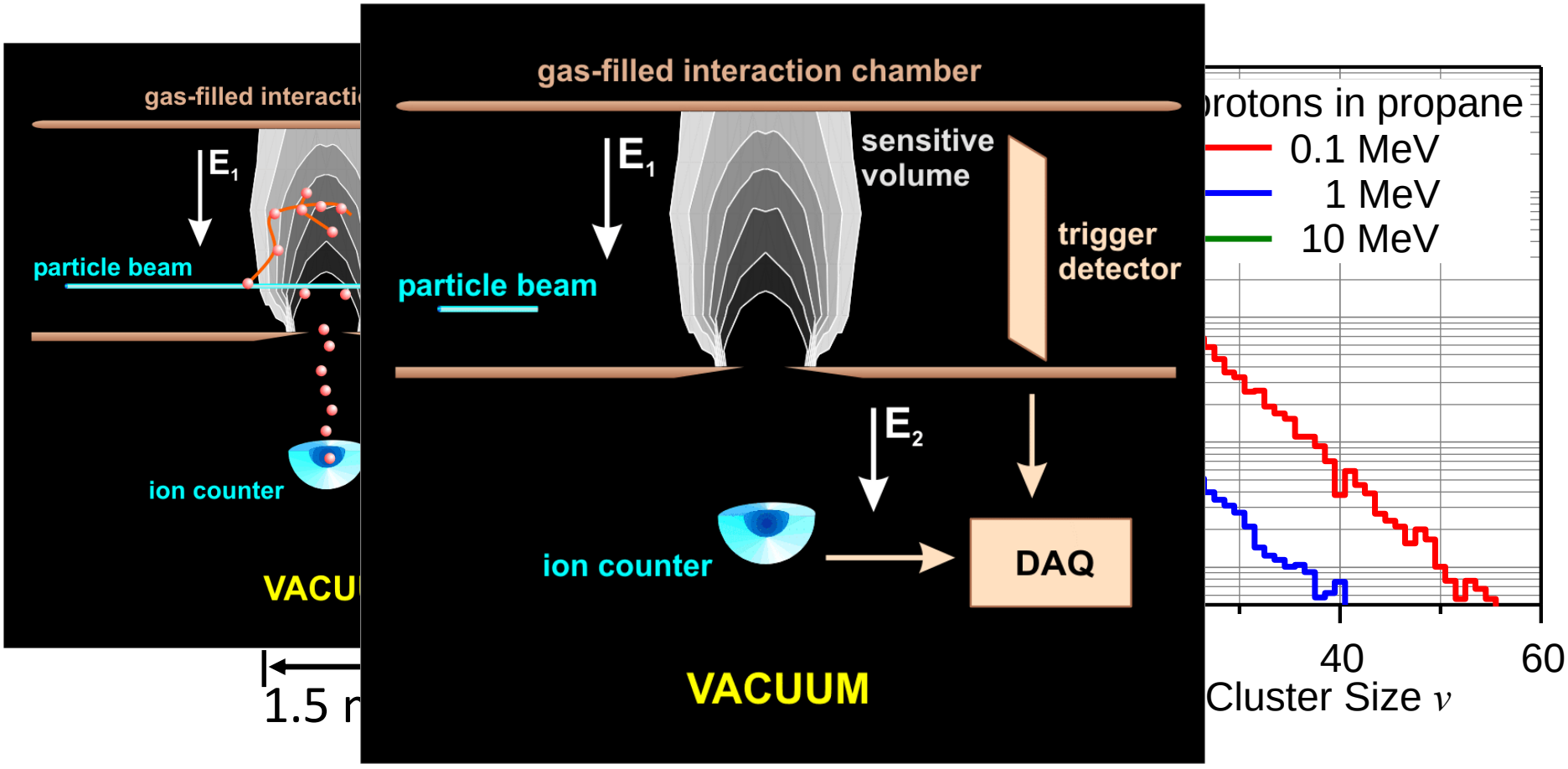
→ Ionisation Cluster Size (ICS)



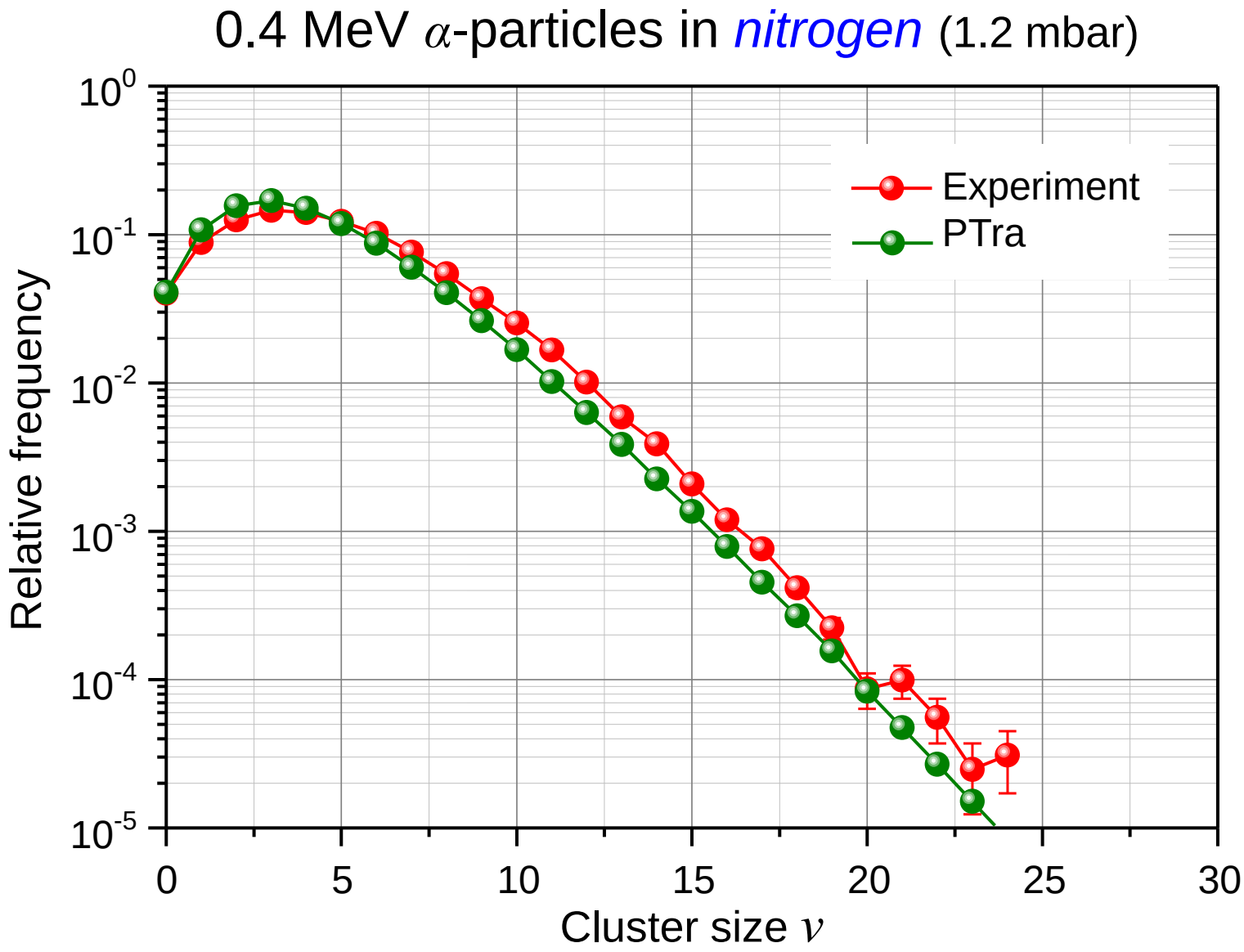
Measuring Ionisation Cluster Size (ICS)

→ Charged particles traverse sensitive volume
→ nitrogen or propane operating gas (low pressure)
→ Ionised gas molecules are extracted, then detected in ion counter

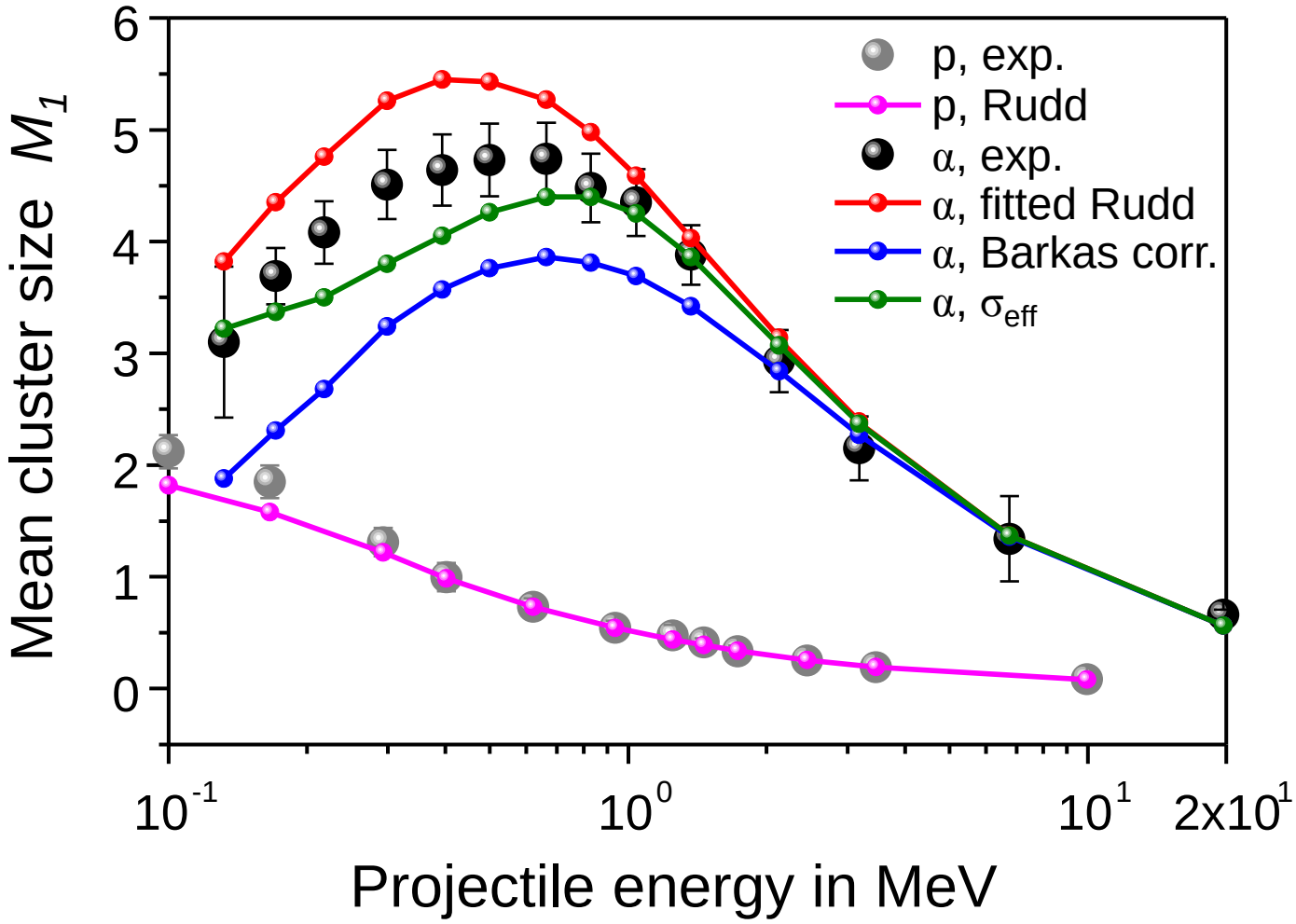
Ion-counting nanodosimeter



Measured vs simulated ICS



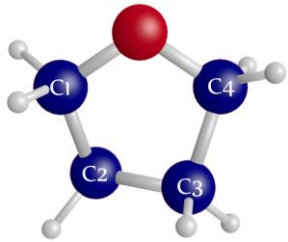
Benchmark: experiments vs PTra simulations



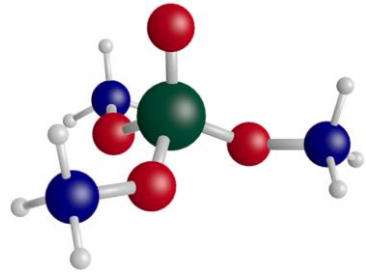
DNA cross sections in Geant4-DNA

Cross sections models of DNA constituents in Geant4-DNA *10.4beta*:

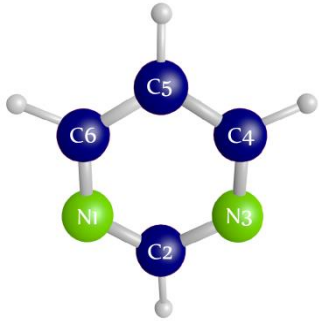
→ THF *(deoxyribose)*, TMP *(phosphates)*, PY *(thymine, cytosine)* and PU *(adenine, guanine)*



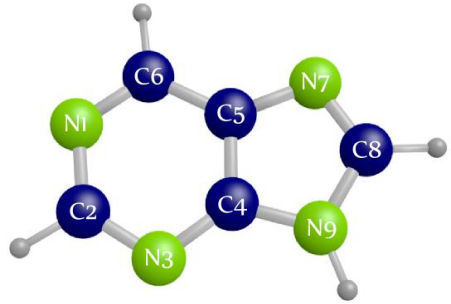
Tetrahydrofuran (THF)



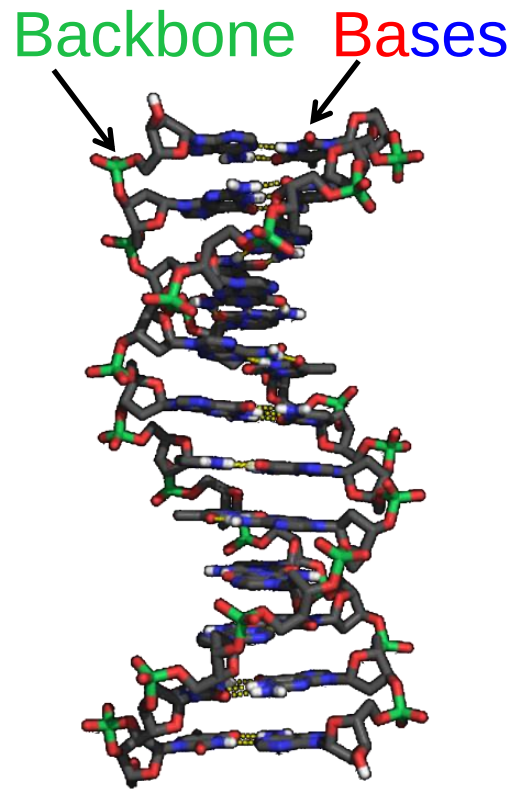
Trimethylphosphate (TMP)



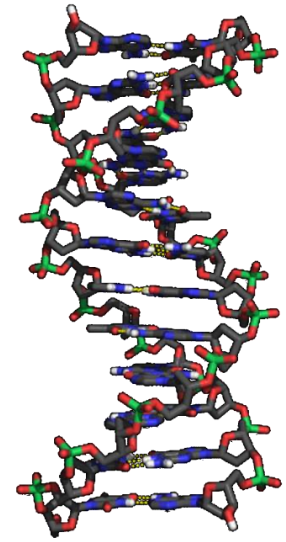
Pyrimidine (PY)



Purine (PU)



DNA cross sections in Geant4-DNA



Structure of new material management system:

→ **G4VDNAModel** class

- Parent class of new material models

→ **G4DNAModelInterface** class

- G4VEmModel similar to that for liquid water
- Register G4VDNAModel classes & combine with existing water models

→ **G4VDNADummyModel** class

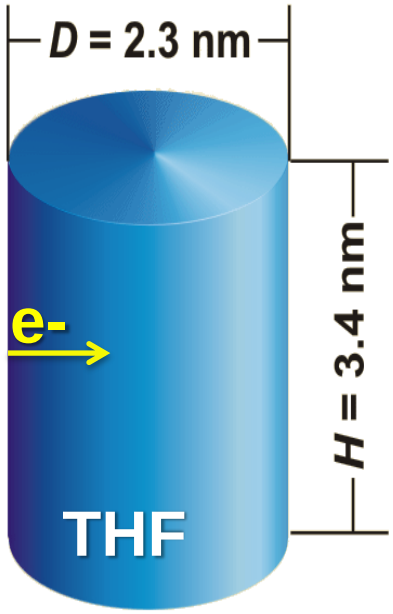
- Transform existing water material *G4VEmModel* into a G4DNAModel
- In order to build mixed materials (water + DNA components)

DNA cross sections in Geant4-DNA

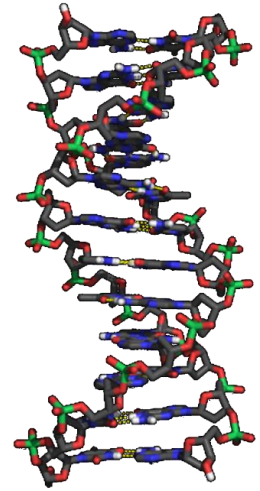
Example with new material management system and DNA cross sections in Geant4 10.4-beta:

/examples/extended/medical/dna/icsd

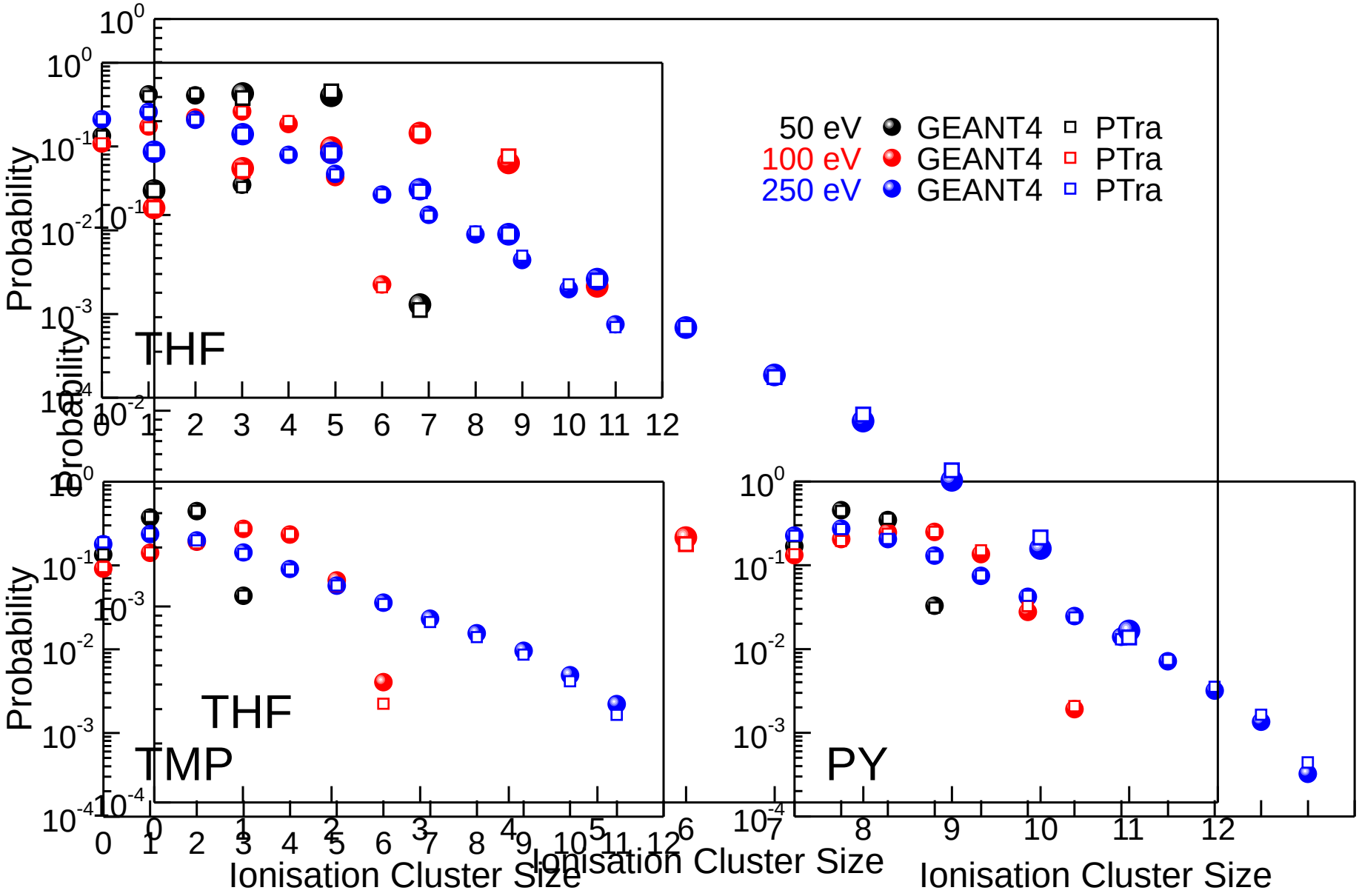
- ICS distribution of 500 eV electrons
- Traversing a cylinder filled with THF surrounded by liquid water



10 base pairs



Geant4-DNA vs PTra simulations: electrons



Proposal: N_2 and C_3H_8 CS in Geant4-DNA

Same approach as that for implementing DNA cross sections:

1) Write new model classes to include cross sections of ***nitrogen*** and ***propane*** gas → G4VDNAModel

2) Initially for electrons, then for ions (H and He)

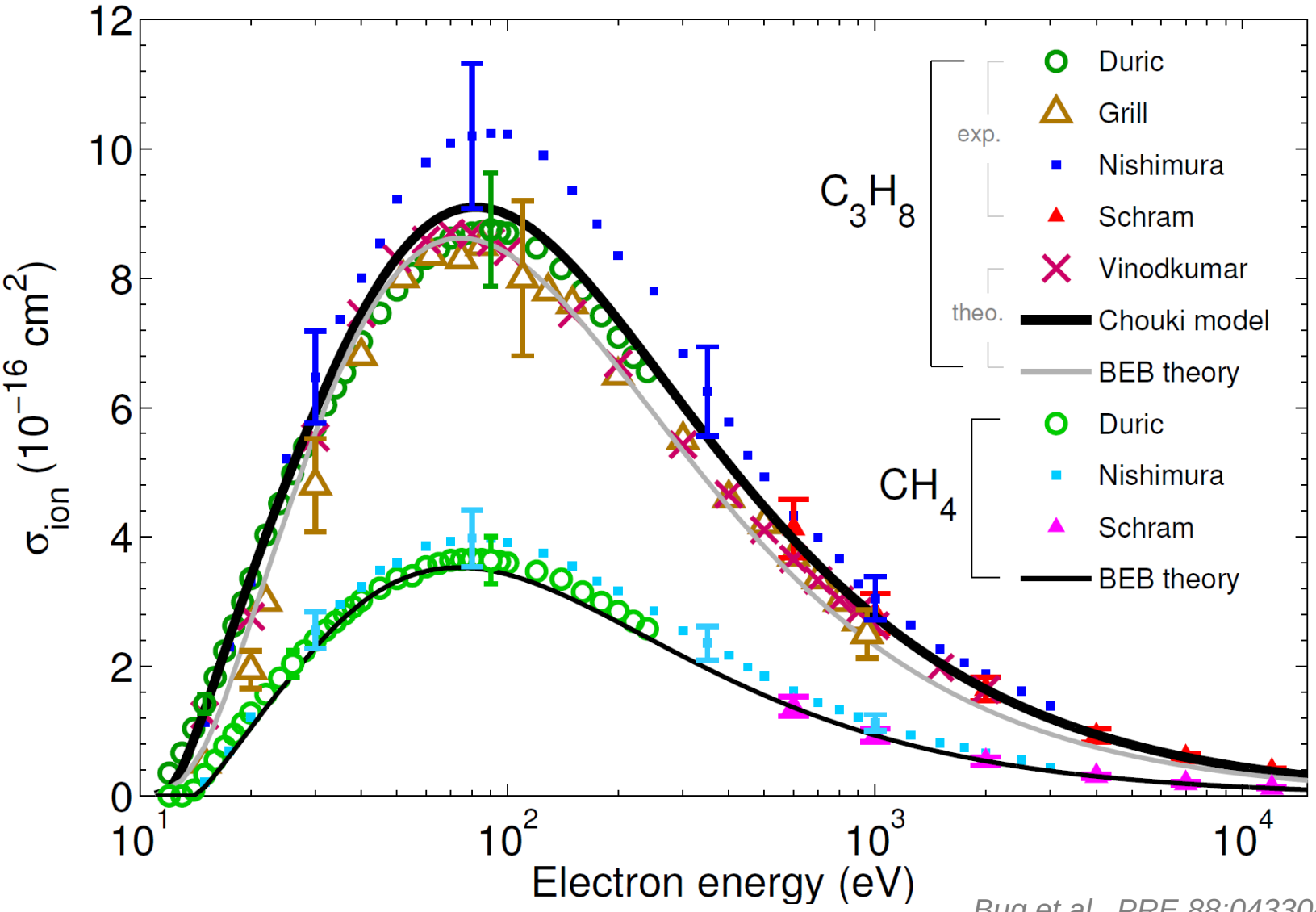
3) Benchmark implemented cross sections:
→ Compare *new version* Geant4-DNA with PTra simulation results

Overview: proposed cross section data

		Nitrogen[§]	Propane[$]
e^-	σ_{el}	Integrated experimental data or screened Rutherford	
	$d\sigma_{el}/d\Omega$	Fitted experimental data or screened Rutherford	
	σ_{ion}	BEB model*	Chouki model*
	$d\sigma_{ion}/dE$	Based on Breit-Wigner distribution (Green and Sawada, 1976)	
	$d^2\sigma_{ion}/dEd\Omega$	Kinematic model (Berger)	
	$\sigma_{exc,j}$	Porter, 1966 adapted to obtain measured TCS	Adapted Chouki model
Ions	σ_{ion}	Rudd model*+	
	$d\sigma_{ion}/dE$	Rudd or HKS model+	
	$d^2\sigma_{ion}/dEd\Omega$	HKS model	
	$\sigma_{exc,j}$	Same as for electrons#	
	Charge transfer	He projectiles: Models for σ_{ion}, charge-transfer, equilibrium fractions*	

§ Grosswendt and Pszona, Rad. Env. Biophys. 41:91 (2002)
$ Grosswendt, Rad. Env. Biophys. 41:103 (2002)
* Bug et al., PRE 88:043308 (2013)
+ Comparison Rudd and HKS models in Gargioni and Grosswendt, NIMA 580:81 (2007)
# Unpublished to date

Electron-impact ionisation CS: *propane*



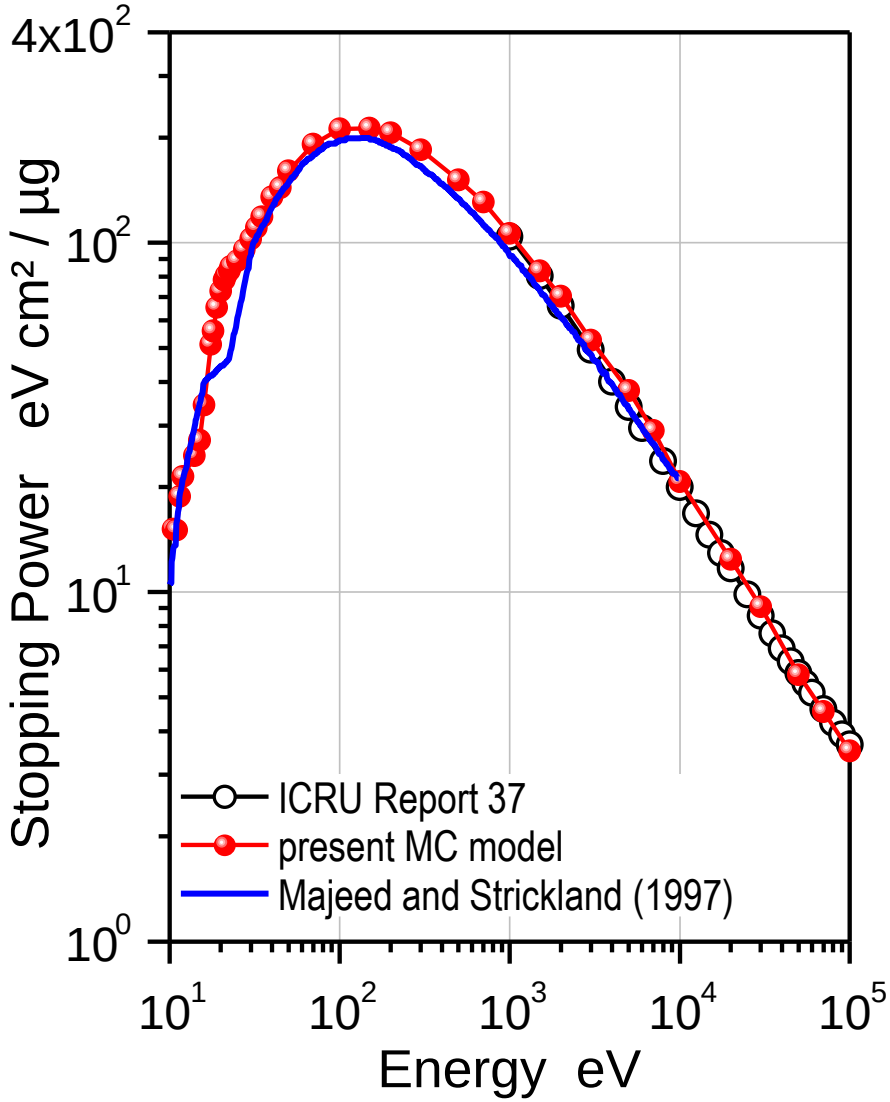
Bug et al., PRE 88:043308 (2013)

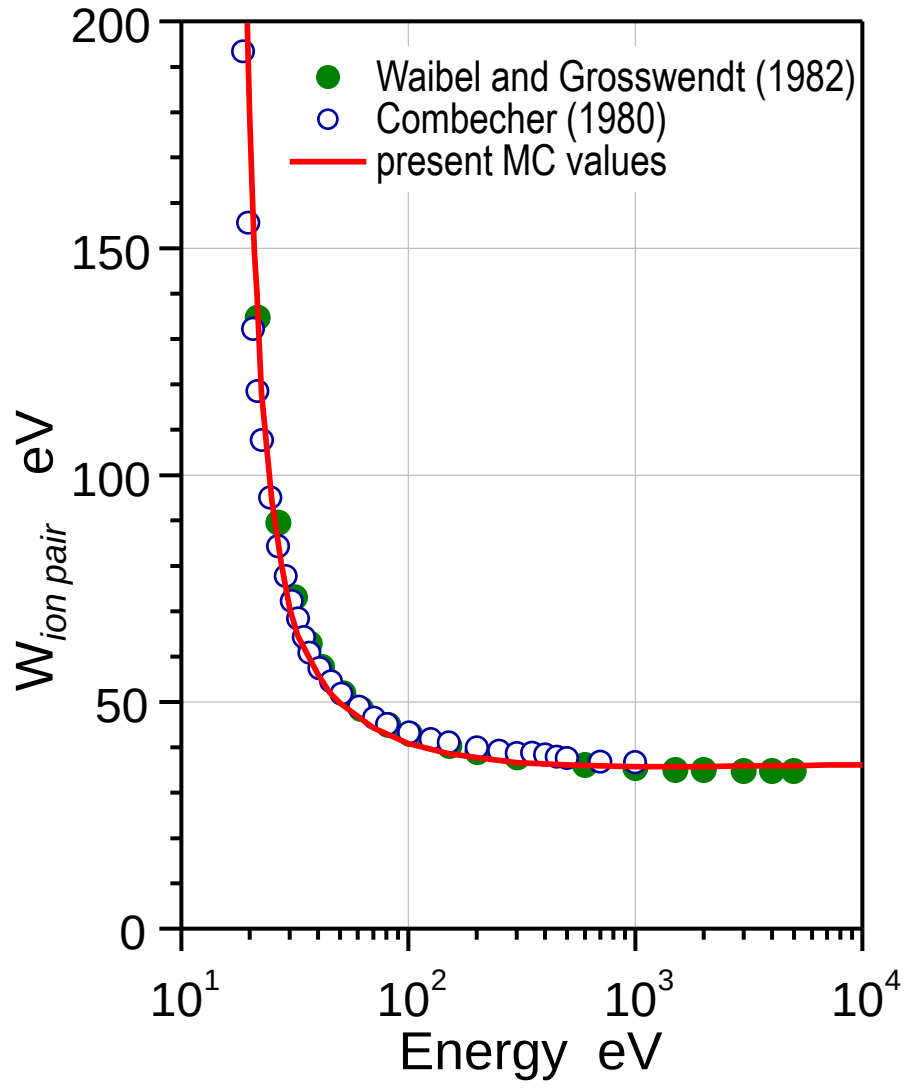
Overview: proposed cross section data

		Nitrogen[§]	Propane[$]
e^-	σ_{el}	Integrated experimental data or screened Rutherford	
	$d\sigma_{el}/d\Omega$	Fitted experimental data or screened Rutherford	
	σ_{ion}	BEB model*	Chouki model*
	$d\sigma_{ion}/dE$	Based on Breit-Wigner distribution (Green and Sawada, 1976)	
	$d^2\sigma_{ion}/dEd\Omega$	Kinematic model (Berger)	
	$\sigma_{exc,j}$	Porter, 1966 adapted to obtain measured TCS	Adapted Chouki model
Ions	σ_{ion}	Rudd model*+	
	$d\sigma_{ion}/dE$	Rudd or HKS model+	
	$d^2\sigma_{ion}/dEd\Omega$	HKS model	
	$\sigma_{exc,j}$	Same as for electrons#	
	Charge transfer	He projectiles: Models for σ_{ion}, charge-transfer, equilibrium fractions*	

§ Grosswendt and Pszona, Rad. Env. Biophys. 41:91 (2002)
$ Grosswendt, Rad. Env. Biophys. 41:103 (2002)
* Bug et al., PRE 88:043308 (2013)
+ Comparison Rudd and HKS models in Gargioni and Grosswendt, NIMA 580:81 (2007)
# Unpublished to date

Verification of CS: e- transport in nitrogen





Grosswendt and Pszona, Rad. Env. Biophys. 41:91 (2002)

Overview: proposed cross section data

		Nitrogen[§]	Propane[$]
e^-	σ_{el}	Integrated experimental data or screened Rutherford	
	$d\sigma_{el}/d\Omega$	Fitted experimental data or screened Rutherford	
	σ_{ion}	BEB model*	Chouki model*
	$d\sigma_{ion}/dE$	Based on Breit-Wigner distribution (Green and Sawada, 1976)	
	$d^2\sigma_{ion}/dEd\Omega$	Kinematic model (Berger)	
	$\sigma_{exc,j}$	Porter, 1966 adapted to obtain measured TCS	Adapted Chouki model
Ions	σ_{ion}	Rudd model*+	
	$d\sigma_{ion}/dE$	Rudd or HKS model+	
	$d^2\sigma_{ion}/dEd\Omega$	HKS model	
	$\sigma_{exc,j}$	Same as for electrons# (of identical velocity)	
	Charge transfer	He projectiles: Models for σ_{ion}, charge-transfer, equilibrium fractions*	

§ Grosswendt and Pszona, Rad. Env. Biophys. 41:91 (2002)
$ Grosswendt, Rad. Env. Biophys. 41:103 (2002)
* Bug et al., PRE 88:043308 (2013)
+ Comparison Rudd and HKS models in Gargioni and Grosswendt, NIMA 580:81 (2007)
# Unpublished to date

Proton-impact ionisation CS: *propane & N_2*

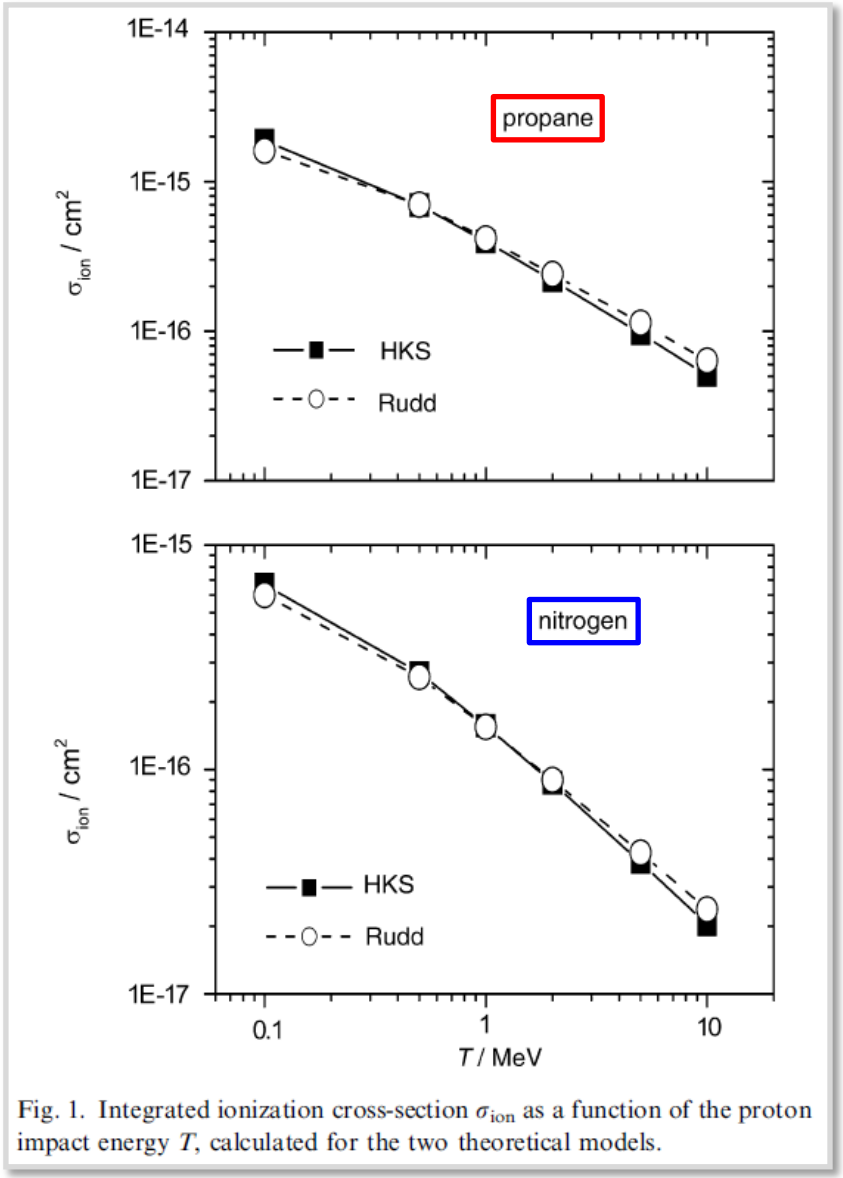


Fig. 1. Integrated ionization cross-section σ_{ion} as a function of the proton impact energy T, calculated for the two theoretical models.

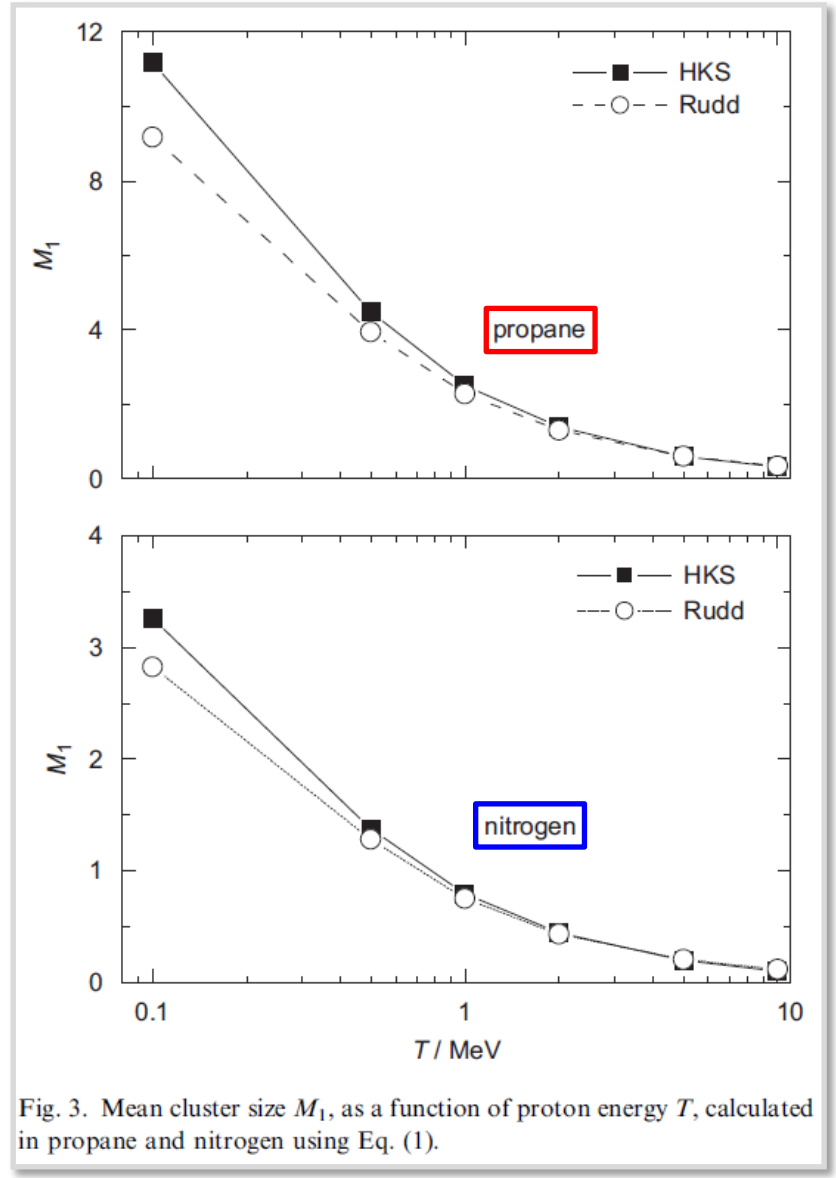


Fig. 3. Mean cluster size M_1, as a function of proton energy T, calculated in propane and nitrogen using Eq. (1).

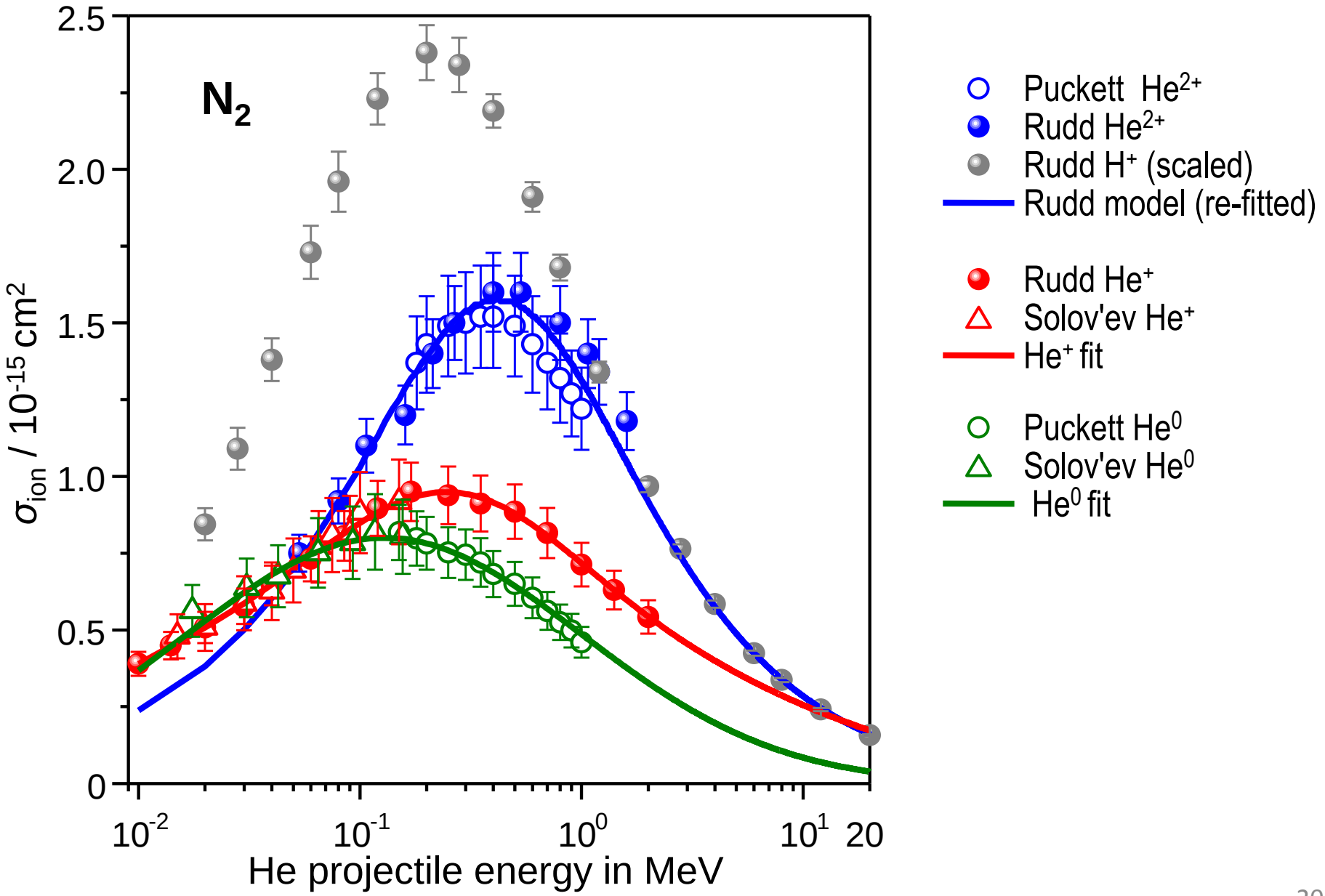
Gargioni and Grosswendt, NIMA 580:81 (2007)

Overview: proposed cross section data

		Nitrogen[§]	Propane[$]
e^-	σ_{el}	Integrated experimental data or screened Rutherford	
	$d\sigma_{el}/d\Omega$	Fitted experimental data or screened Rutherford	
	σ_{ion}	BEB model*	Chouki model*
	$d\sigma_{ion}/dE$	Based on Breit-Wigner distribution (Green and Sawada, 1976)	
	$d^2\sigma_{ion}/dEd\Omega$	Kinematic model (Berger)	
	$\sigma_{exc,j}$	Porter, 1966 adapted to obtain measured TCS	Adapted Chouki model
Ions	σ_{ion}	Rudd model*+	
	$d\sigma_{ion}/dE$	Rudd or HKS model+	
	$d^2\sigma_{ion}/dEd\Omega$	HKS model	
	$\sigma_{exc,j}$	Same as for electrons# (of identical velocity)	
	Charge transfer	He projectiles: Models for σ_{ion}, charge-transfer, equilibrium fractions*	

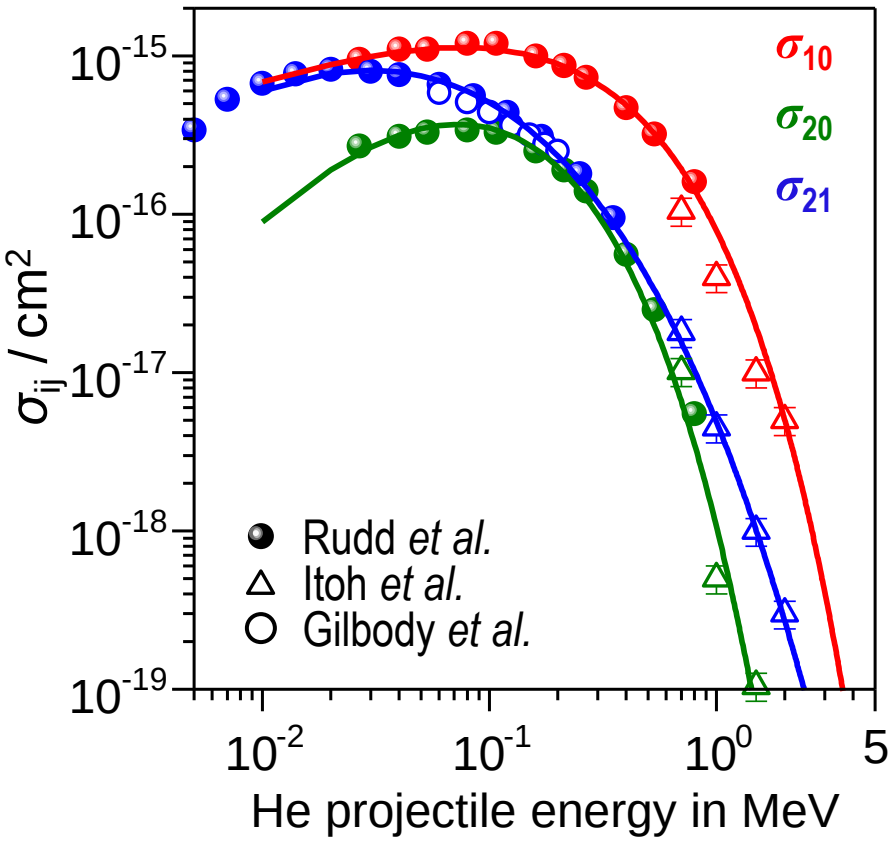
§ Grosswendt and Pszona, Rad. Env. Biophys. 41:91 (2002)
$ Grosswendt, Rad. Env. Biophys. 41:103 (2002)
* Bug et al., PRE 88:043308 (2013)
+ Comparison Rudd and HKS models in Gargioni and Grosswendt, NIMA 580:81 (2007)
# Unpublished to date

Helium-impact ionisation CS: *nitrogen*

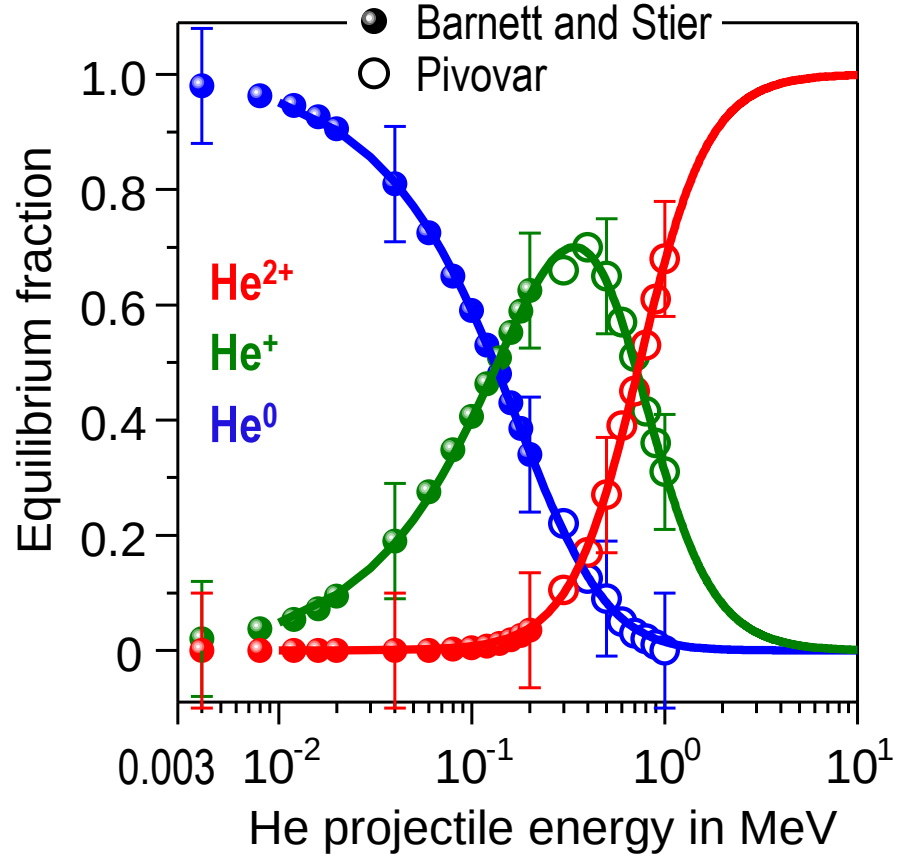


Helium charge-transfer CS: *nitrogen*

Electron-capture CS



Equilib. fractions of charge states



Equilibrium condition: $f_i\sigma_{ij} = f_j\sigma_{ji}$

Overview: proposed cross section data

		Nitrogen[§]	Propane[$]
e^-	σ_{el}	Integrated experimental data or screened Rutherford	
	$d\sigma_{el}/d\Omega$	Fitted experimental data or screened Rutherford	
	σ_{ion}	BEB model*	Chouki model*
	$d\sigma_{ion}/dE$	Based on Breit-Wigner distribution (Green and Sawada, 1976)	
	$d^2\sigma_{ion}/dEd\Omega$	Kinematic model (Berger)	
	$\sigma_{exc,j}$	Porter, 1966 adapted to obtain measured TCS	Adapted Chouki model
Ions	σ_{ion}	Rudd model*+	
	$d\sigma_{ion}/dE$	Rudd or HKS model+	
	$d^2\sigma_{ion}/dEd\Omega$	HKS model	
	$\sigma_{exc,j}$	Same as for electrons# (of identical velocity)	
	Charge transfer	He projectiles: Models for σ_{ion}, charge-transfer, equilibrium fractions*	

§ Grosswendt and Pszona, Rad. Env. Biophys. 41:91 (2002)
$ Grosswendt, Rad. Env. Biophys. 41:103 (2002)
* Bug et al., PRE 88:043308 (2013)
+ Comparison Rudd and HKS models in Gargioni and Grosswendt, NIMA 580:81 (2007)
# Unpublished to date

Summary

- Cross section models of **DNA** constituents for electrons and ions have been implemented into Geant4-DNA *10.4beta*

- Proposed further development: implement **propane** and **nitrogen** cross sections for electrons & ions into Geant4-DNA

  → Benchmark with the PTra code

- Extend the use of Geant4-DNA to applications and users in the micro- and nanodosimetry community