



TOR VERGATA
UNIVERSITÀ DEGLI STUDI DI ROMA

Thermal neutron cross-sections of air: the contribution of molecular rotations

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PRESENTATION AGENDA

- 1 The role of neutrons in medical physics
- 2 Thermal neutrons interactions
- 3 Thermal neutron cross section of air
- 4 Measuring neutron cross section of air
- 5 Conclusion and outlook

The role of neutrons in medical physics

- Neutral particles: can penetrate deeply
- Very sensitive to hydrogen
- **Neutrons can activate other atoms!**

Pro: Can be used to produce medical **radioisotopes**

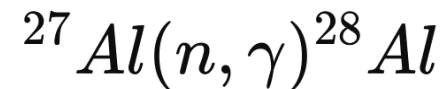
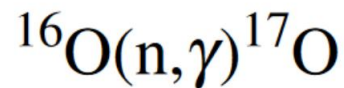
Cons: Risk of **secondary dose** to the patient

Neutrons can activate:

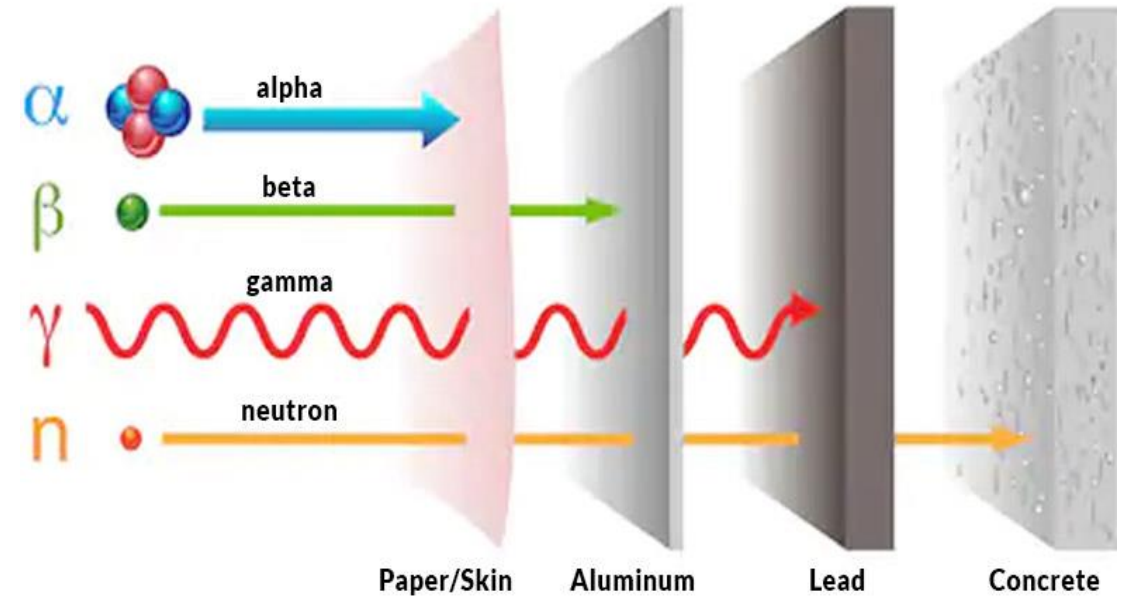
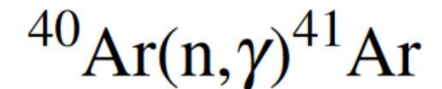
- Atoms inside the patient



- Atoms in medical equipment and shielding



- Atoms in air!



The role of neutrons in medical physics

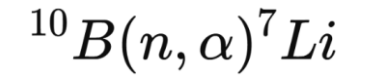
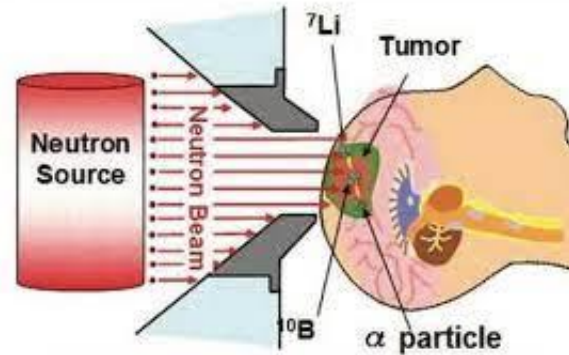
LINAC for radiotherapy



Secondary neutrons produced by photoproduction

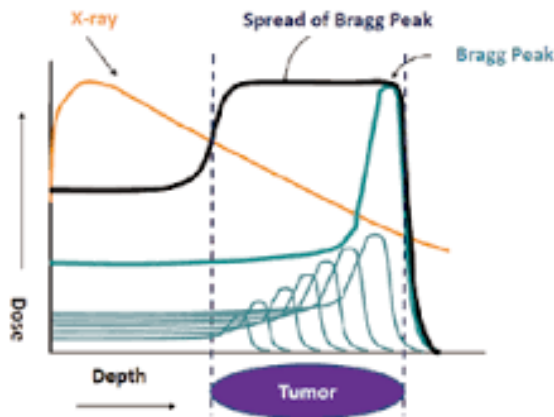
Reaction	Threshold (Mev)
N-14(γ ,n)N-13	10.55
O-16(γ ,n)O-15	15.67
C-12(γ ,n)C-11	18.72

Neutron capture therapy



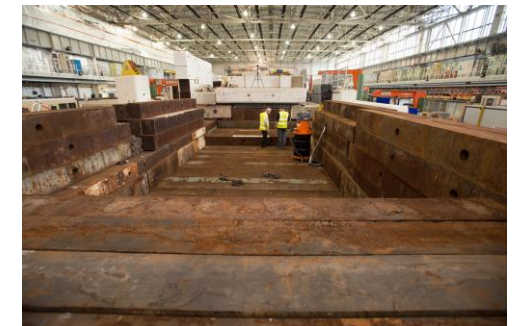
Reaction products destroy cancer cells

Proton therapy



Neutron dose is negligible when using a pencil proton beam, but not with passively scattered proton beams.

Radiation protection safety measures in other applications:



The role of neutrons in medical physics

Thermal neutron Cross Sections (TCSs) are a fundamental ingredient for the simulation and design of medical equipment

Safety measures have to be tailored to each specific case, taking into account both the **medical device** and its **sorroundings**

Simulations are performed to establish both **design** and **operating mode** of the device

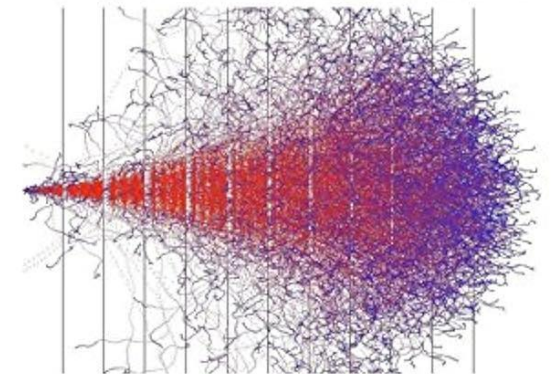
Monte Carlo transport simulations



MC codes require accurate models for particle **cross sections**

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{\text{neutrons scattered per second}}{\Phi(E)d\Omega dE'}$$

Monte Carlo Methods for Particle Transport



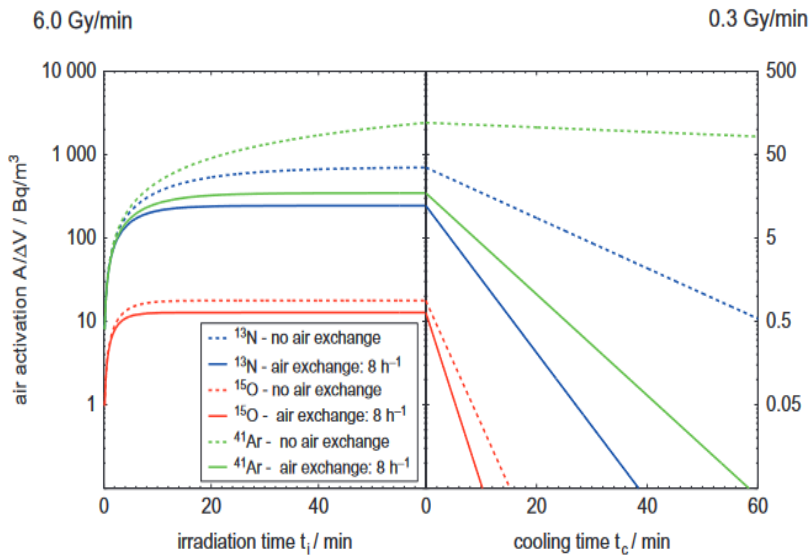
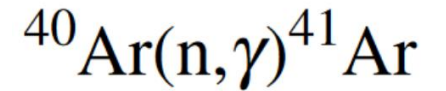
Alireza Haghightat

CRC Press
Taylor & Francis Group

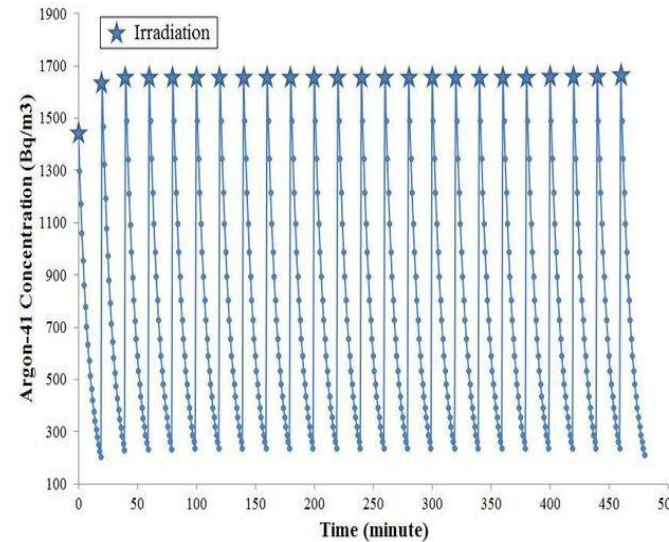
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The role of neutrons in medical physics

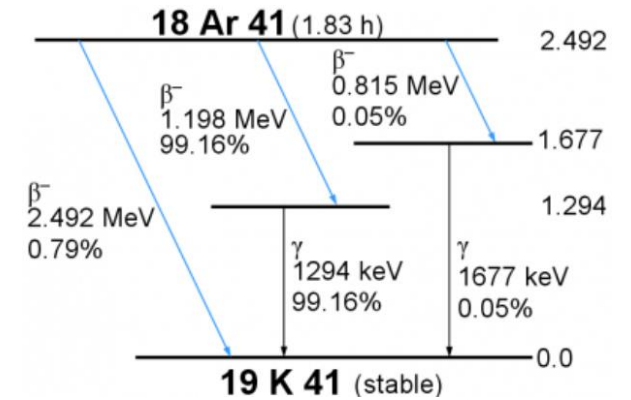
When operating a LINAC air activation needs to be taken into account



“On the neutron radiation field and air activation around a medical electron linac” Felix Horst et al. (2016)



Latifah, R & Bunawas, & Noor, Johan. (2018). The estimation of occupational dose in 15 MV varian clinac ix room by Argon-41 as an activation product of photoneutron. Journal of Physics: Conference Series



Barker JG, Mildner DF. Survey of background scattering from materials found in small-angle neutron scattering. J Appl Crystallogr. 2015

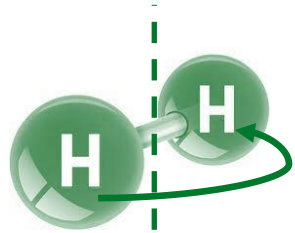
Discrepancies with experimental results are often attributed to uncertainties of air humidity, however, **molecular motion is not taken into account!**



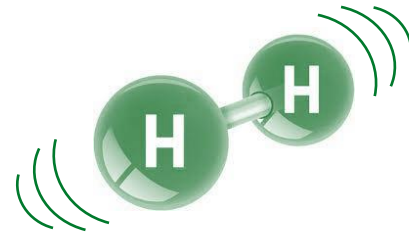
Thermal neutrons interactions

The cross section of diatomic molecules such as N_2 and O_2 depends on multiple degrees of freedom, and is not well approximated by a free gas model. Diatomic molecules can:

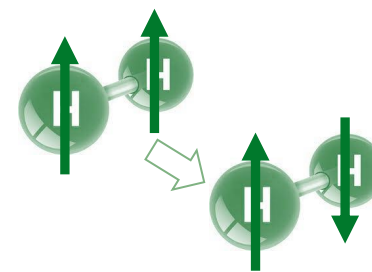
rotate about their centre of mass



vibrate along their axis



flip their spin

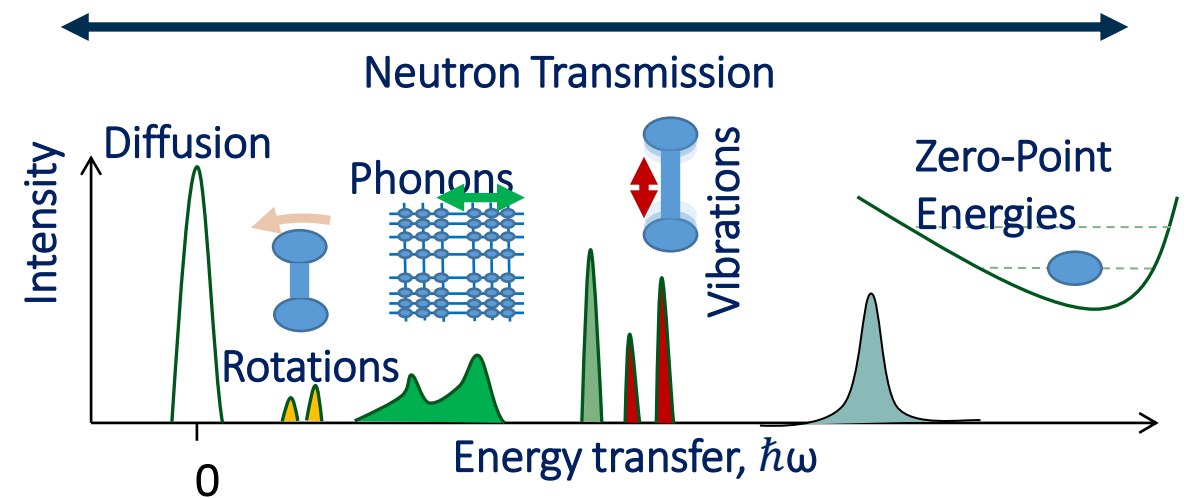


and move in space



The cross section of diatomic molecules can be calculated using the **Young and Koppel model**

J. A. Young and J. U. Koppel. Slow neutron scattering by molecular hydrogen and deuterium. *Phys. Rev.*, 135:A603–A611, Aug 1964.

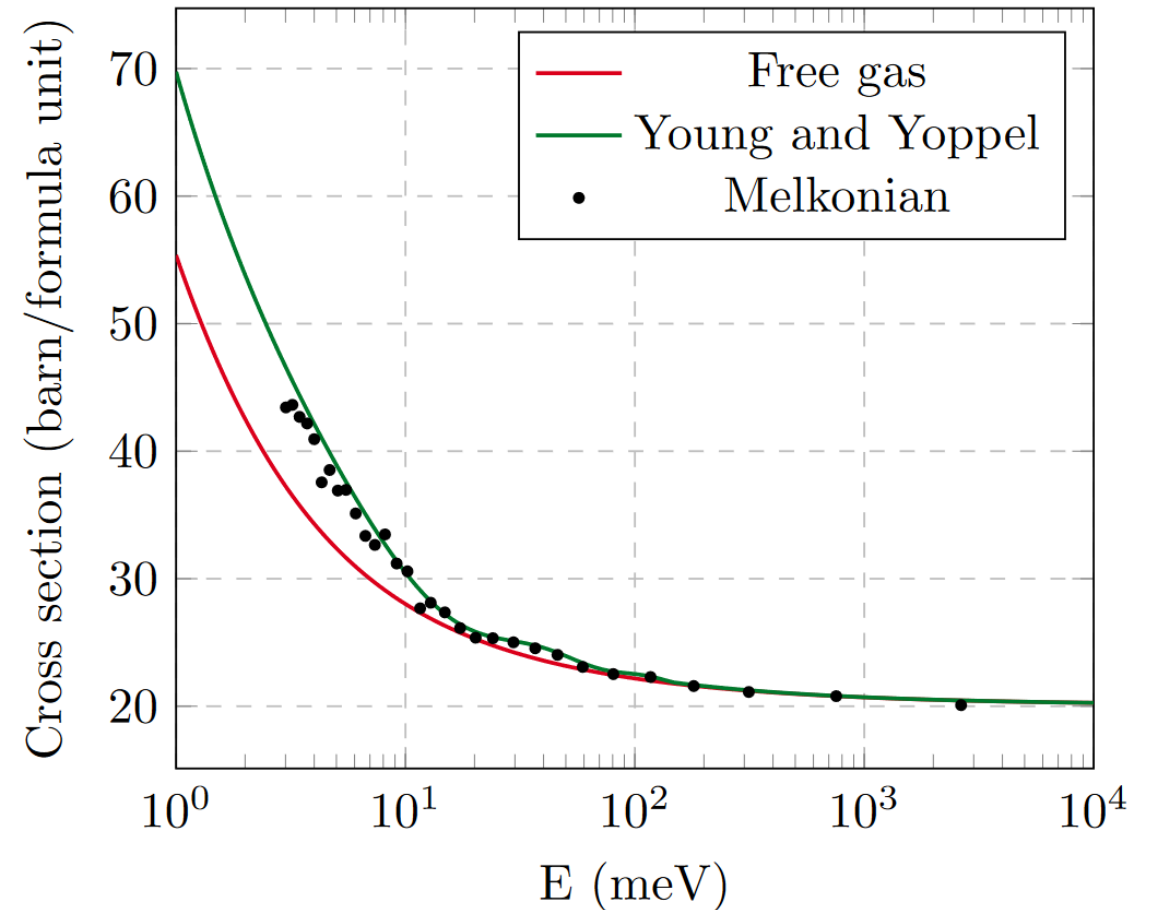


Thermal neutron cross section of N_2

We performed the calculation of thermal neutron cross section of diatomic molecules that are abundant in air

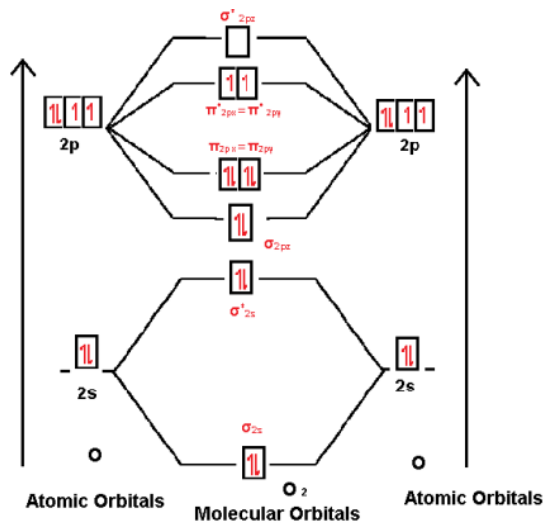
Neutron scattering cross section was estimated using **Young and Koppel model**, and compared to the free gas model and to experimental data from 1955.

Melkonian, E. Slow neutron velocity spectrometer studies of O_2 , N_2 , Ar , H_2 , H_2O , and seven hydrocarbons. Phys. Rev. 76, 1750–1759

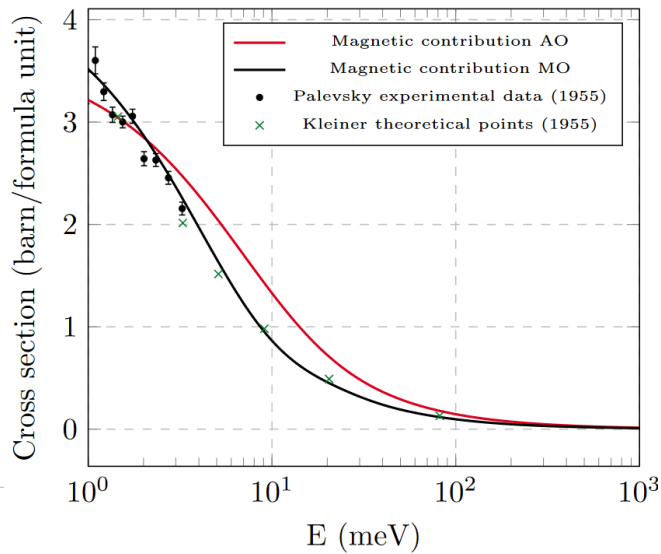


Thermal neutron cross section of O_2

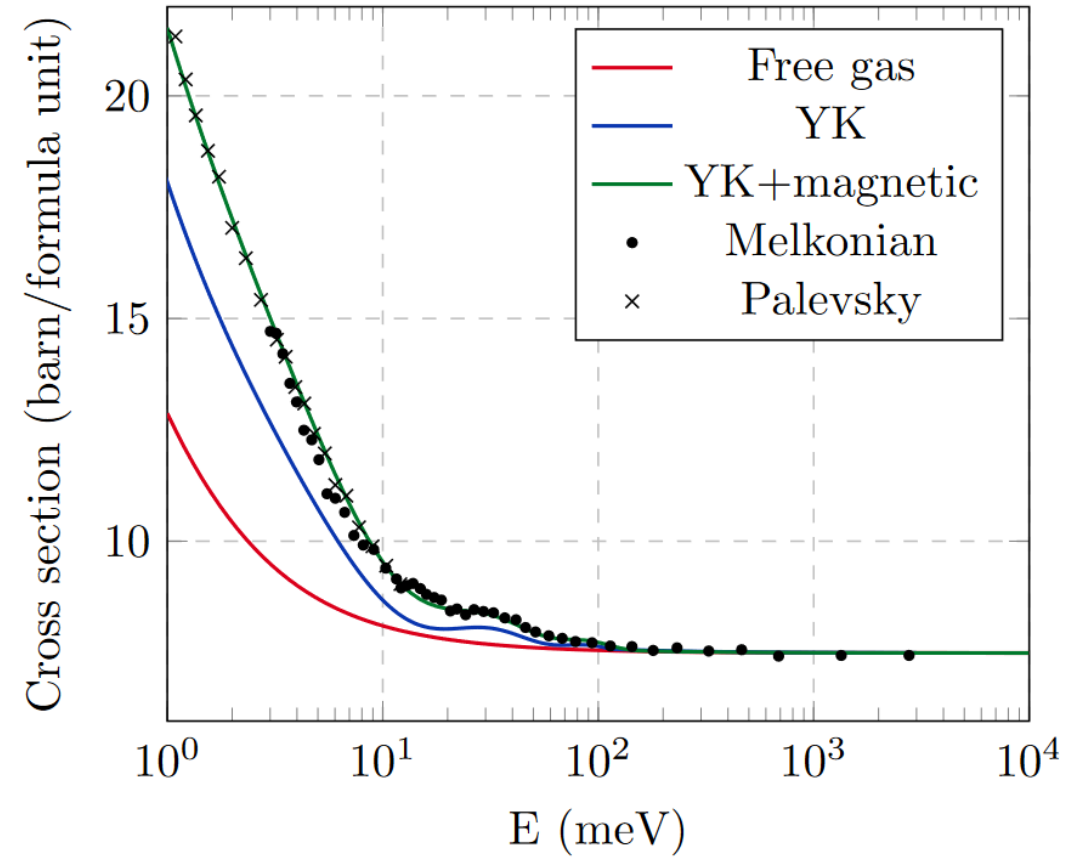
Young and Koppel model was not enough to reproduce O_2 cross section: Its paramagnetic behaviour need to be considered.



Magnetic Scattering of Slow Neutrons from O_2 Gas Kleiner, W. H. Phys. Rev 1955



Molecular Oxygen



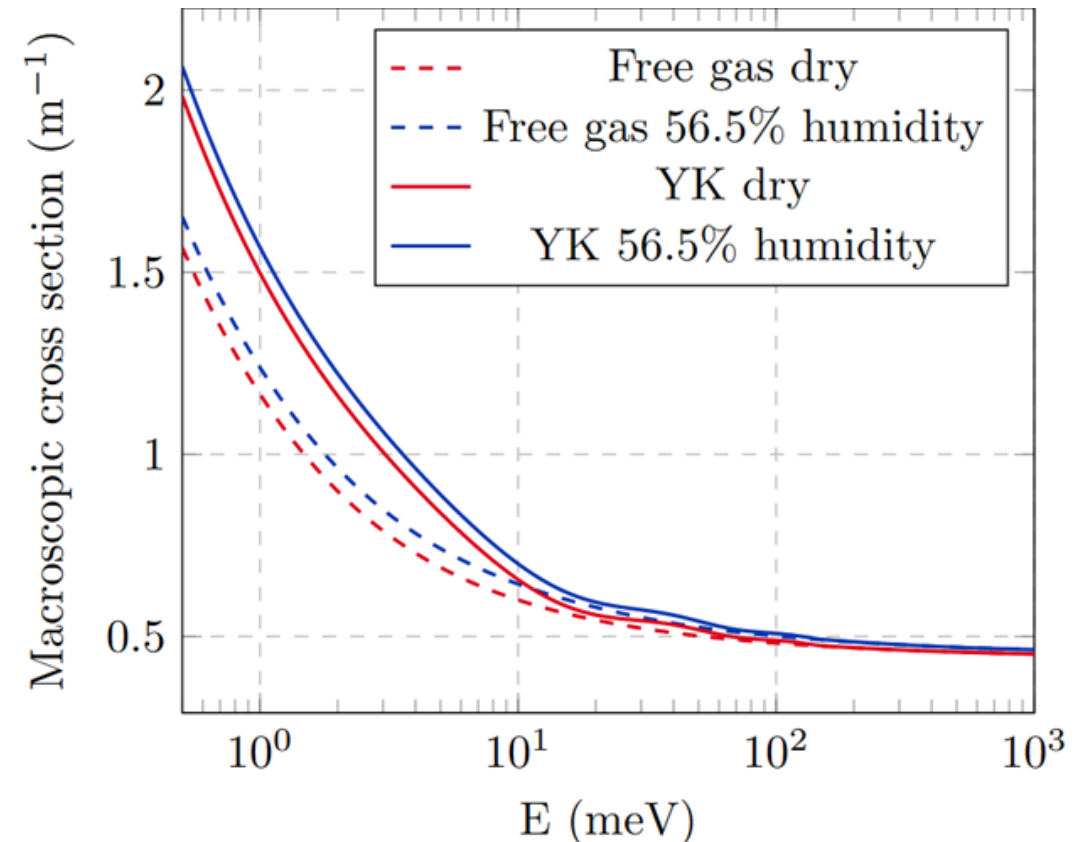
Thermal neutron cross section of air

Air composition was approximated as:

Isotope	mol% in dry air	mol% in hydrated air	Reaction	Absorption XS (barn)
^{14}N	0.7848	0.7696	$^{14}\text{N}(n,\gamma)^{15}\text{N}$ $^{14}\text{N}(n,p)^{14}\text{C}$	0.075 1.84
^{16}O	0.2105	0.2064 in O_2 0.0065 in H_2O	$^{16}\text{O}(n,\gamma)^{17}\text{O}$	0.0001
^{40}Ar	0.0047	0.0046	$^{40}\text{Ar}(n,\gamma)^{41}\text{Ar}$	0.66
^1H	0	0.0129	$^1\text{H}(n,\gamma)^2\text{H}$	0.3326

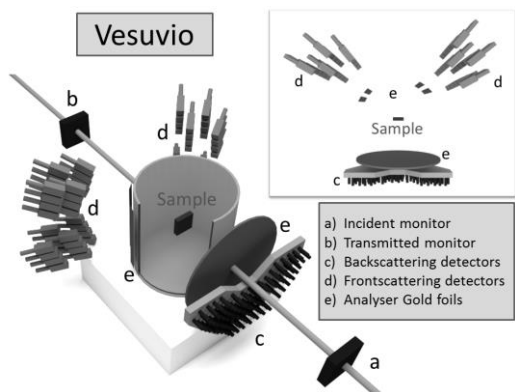
- Mole fraction of water vapour was calculated according to appendix A.1 of <https://www.nist.gov/system/files/documents/calibrations/CIPM-2007.pdf>

Parameter	Value
Air Density	0.001225 g/cm^3
Humidity	56.5 %
Pressure	$1.013 \times 10^5 \text{ Pa}$
Temperature	293.6 K



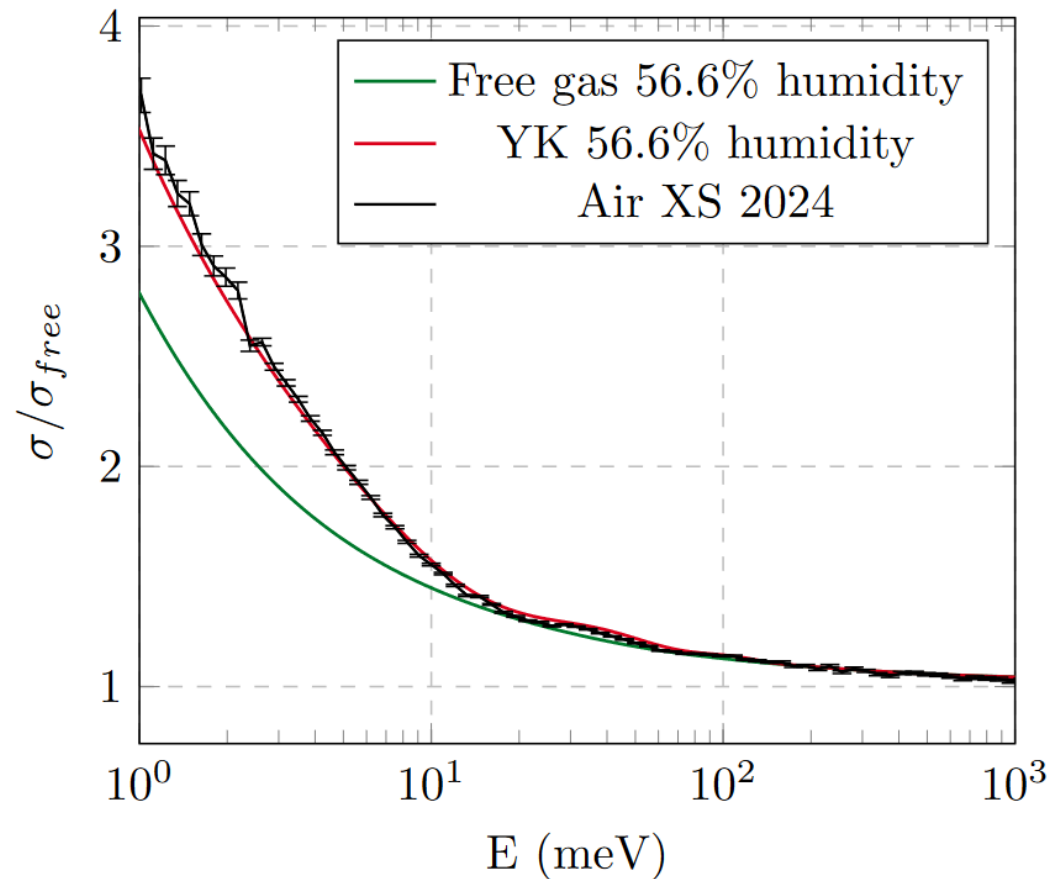
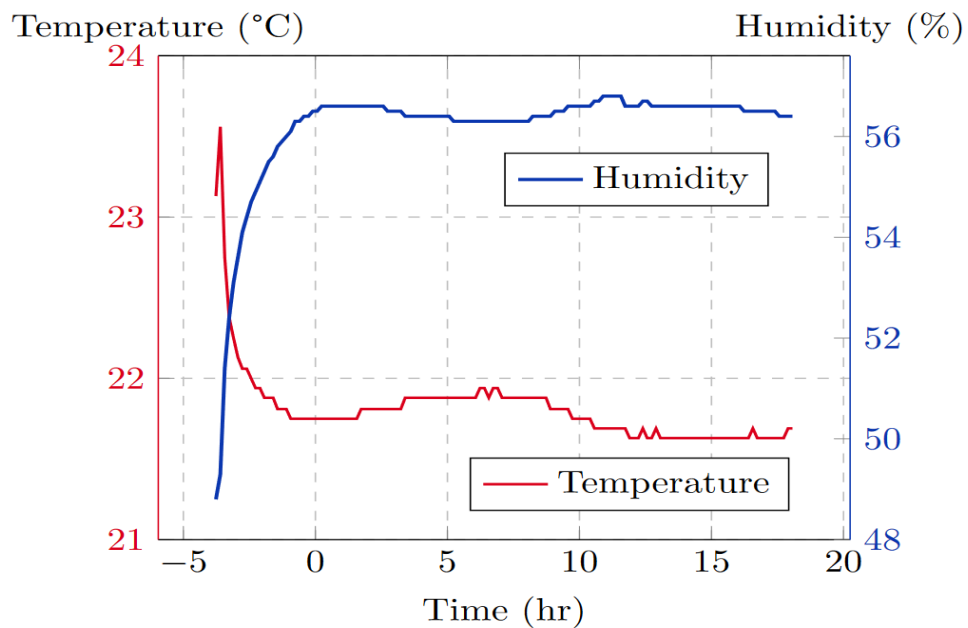
We found that air cross section is strongly affected by molecular rotations!

Measuring neutron cross section of air



VESUVIO spectrometer was employed to perform transmission measurements

Experimental results are in good agreement with our model



Conclusions and outlook

- The Young and Koppel model, together with the paramagnetic model, proved to better estimate the Total cross section of Air at a given humidity percentage.
- This model will be used in Geant 4 transport simulations with the use of the Ncrystal toolkit, to establish its impact on Ar-40 activation.

Aknowledgments:



