Calculating subsurface nucleonic production of noble gas nuclides: implications on crustal and mantle K, Th, U abundances

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Collaboration with
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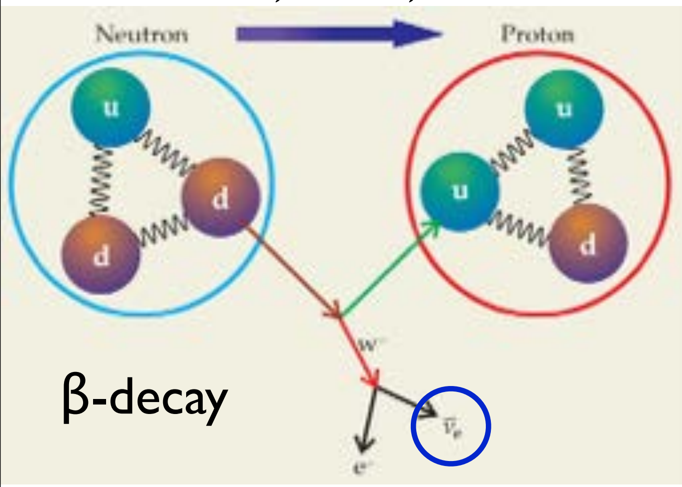
presented at Geophysics Department, Charles University in Prague on Dec 16, 2013

How much radiogenic heating in the mantle??

What is the Earth made of??

Chemical reservoirs in the mantle??

^{238}U, ^{232}Th, ^{40}K



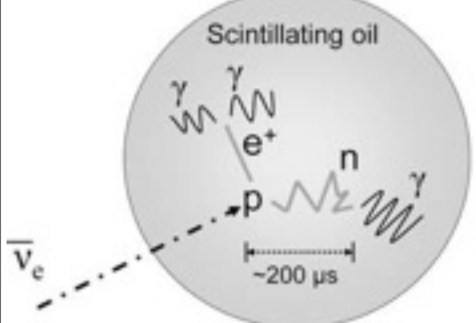
β-decay

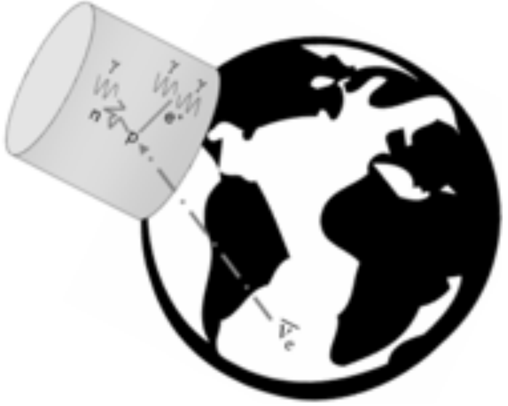
Geoneutrinos:
electron antineutrinos emitted in β-decays of natural radionuclides

$$
\begin{aligned}
{}^{238}_{92}\mathrm{U} &\longrightarrow {}^{206}_{82}\mathrm{Pb} + 8\alpha + 6e^- + \boxed{6\bar{\nu}_e} + 51.698\,\mathrm{MeV}\\
{}^{235}_{92}\mathrm{U} &\longrightarrow {}^{207}_{82}\mathrm{Pb} + 7\alpha + 4e^- + \boxed{4\bar{\nu}_e} + 46.402\,\mathrm{MeV}\\
{}^{232}_{90}\mathrm{Th} &\longrightarrow {}^{208}_{82}\mathrm{Pb} + 6\alpha + 4e^- + \boxed{4\bar{\nu}_e} + 42.652\,\mathrm{MeV}\\
{}^{40}_{19}\mathrm{K} &\xrightarrow{89.3\,\%} {}^{40}_{20}\mathrm{Ca} + e^- + \boxed{\bar{\nu}_e} + 1.311\,\mathrm{MeV},
\end{aligned}
$$

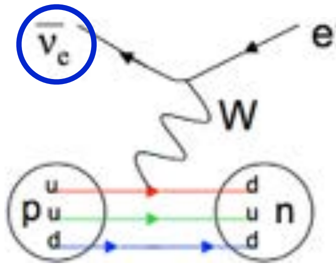
Geo-ν detection possible:

Large liquid scintillator detectors

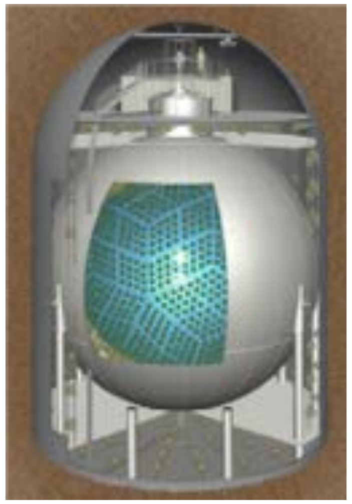




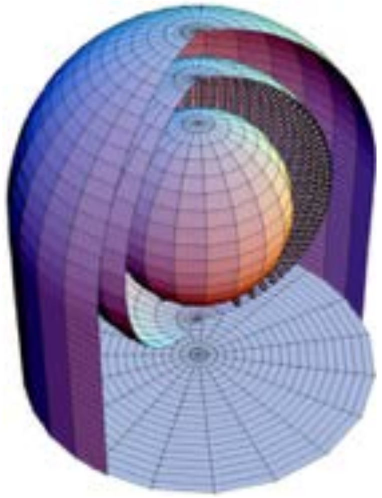
Direct information on Earth's deep-seated radioactivity!



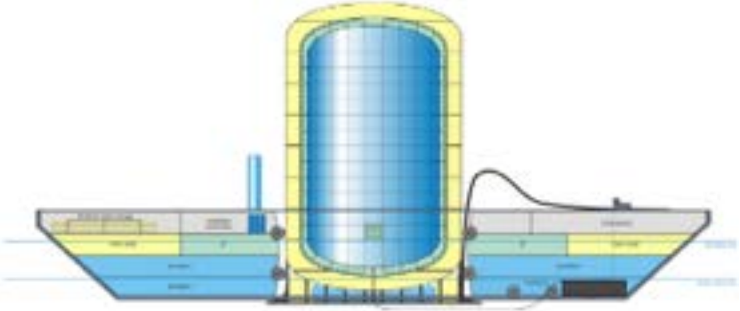
KamLAND (Japan)



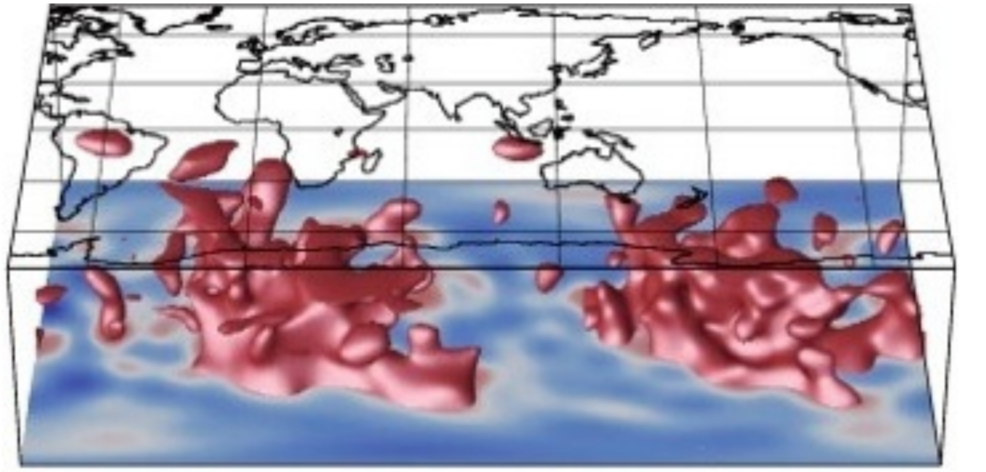
Borexino (Italy)



Hanohano, proposed ocean deployment

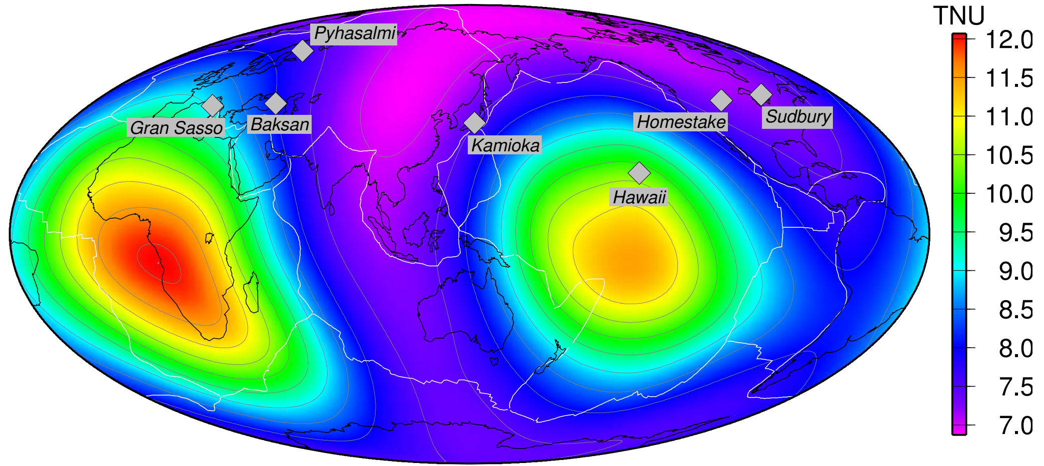


LLSVPs may represent material enriched in U, Th, K



from Bull et al. 2009

Predicted mantle geoneutrino flux

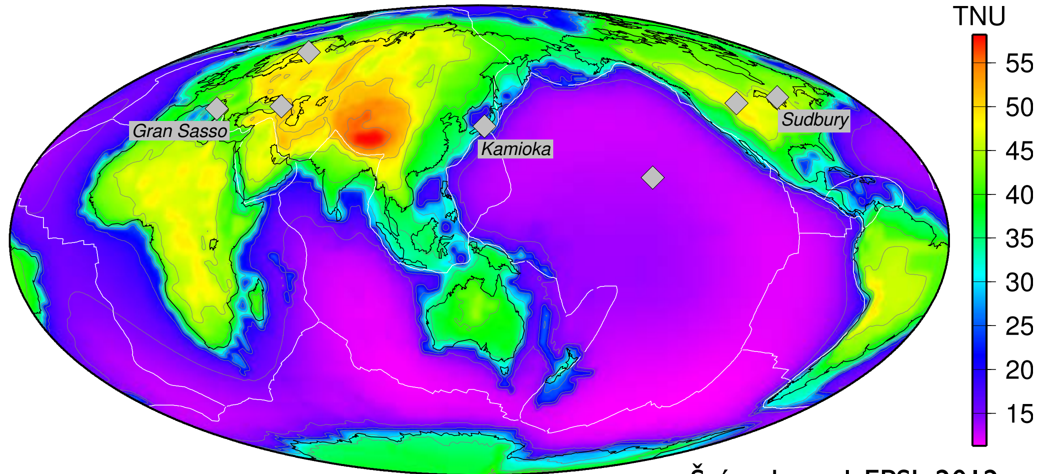


Šrámek et al. EPSL 2012

Mantle: detectable variation!

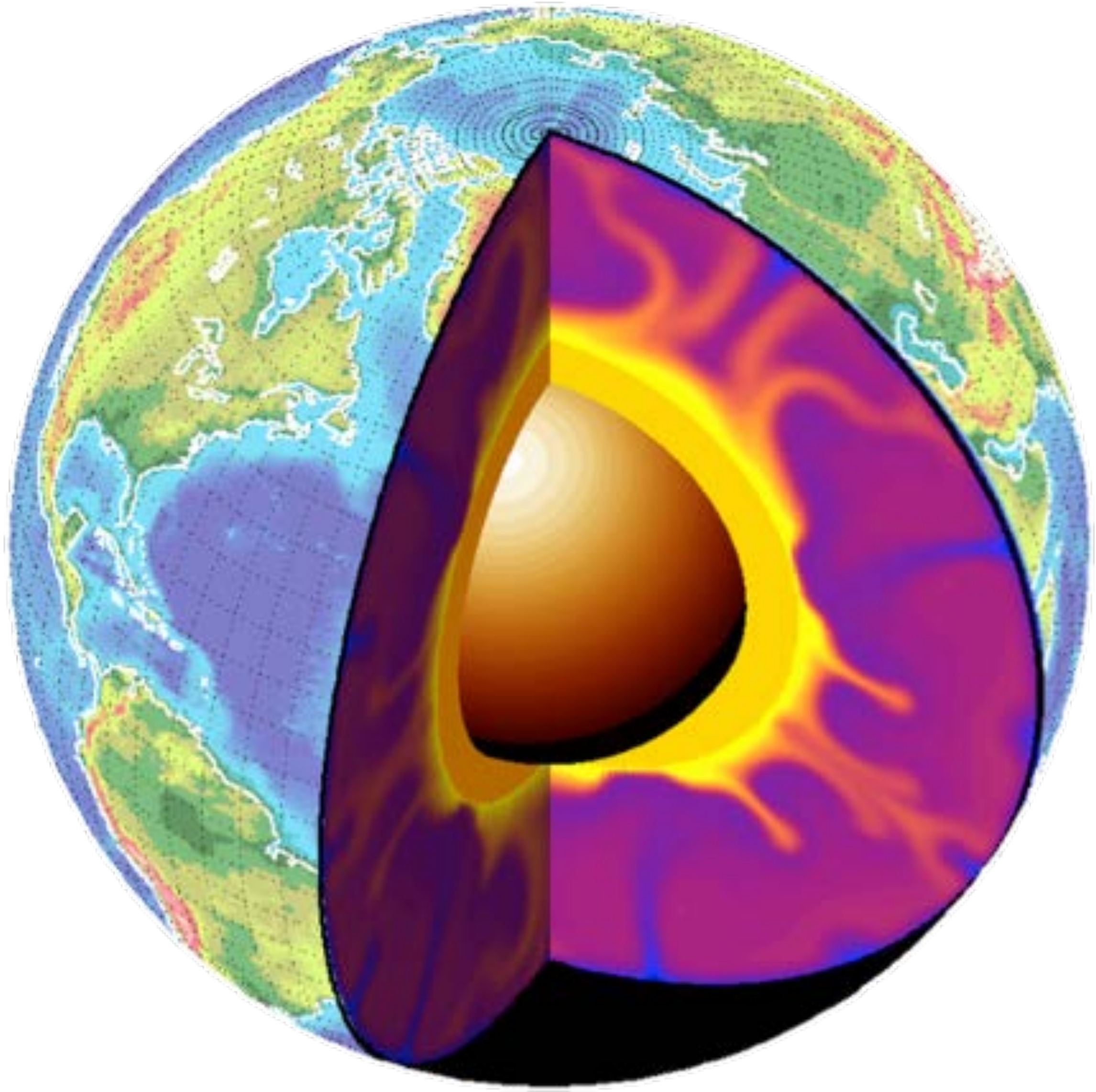
Must measure in the ocean...

Crust + mantle geoneutrino flux



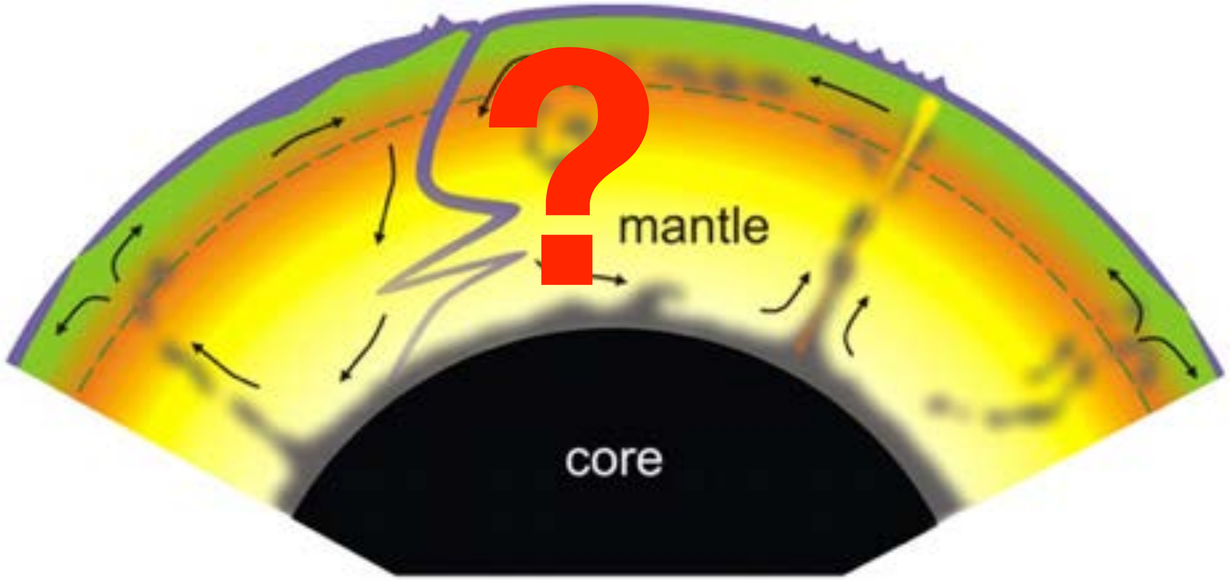
Šrámek et al. EPSL 2012

How much U, Th, K in the Earth?



Estimates range from 9 to 36 TW radiogenic power

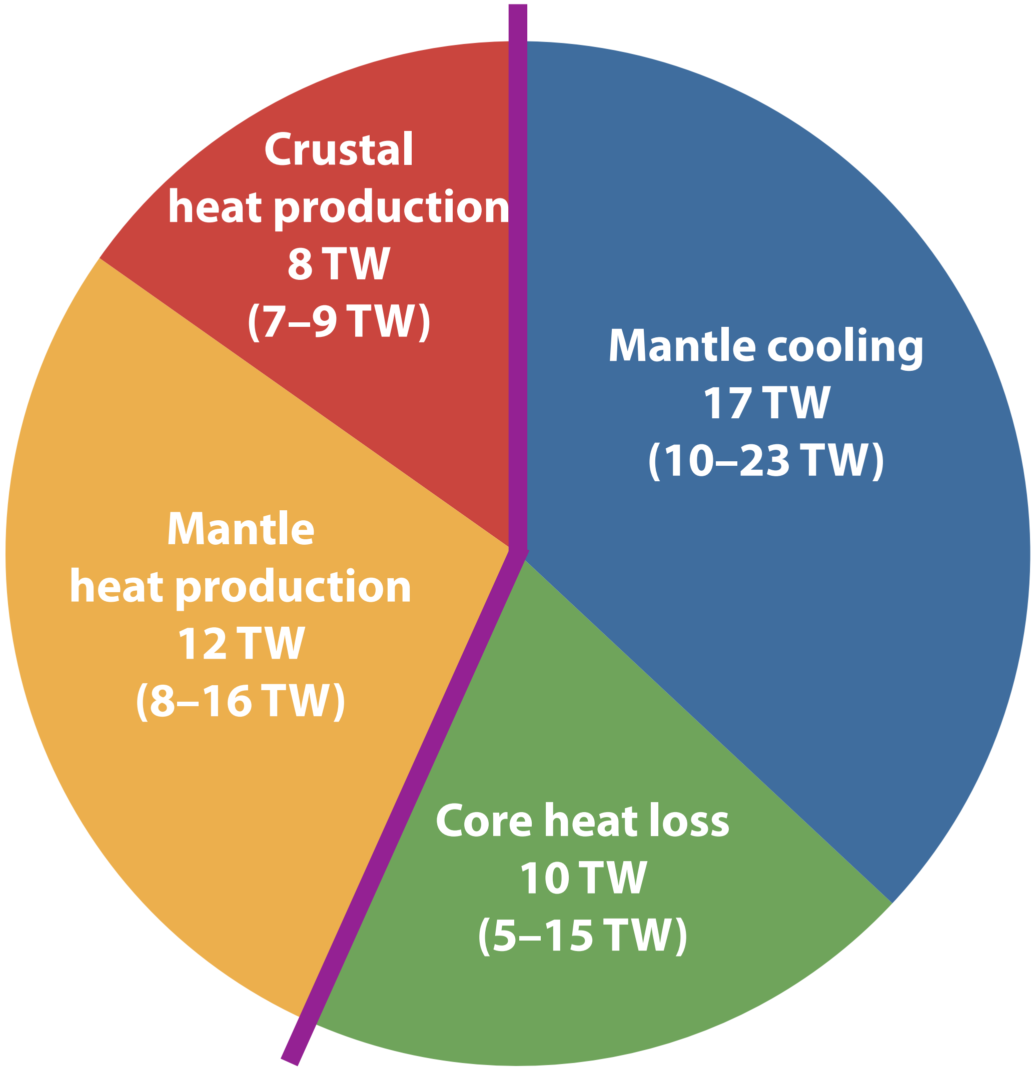
How much radiogenic heating in the mantle to power convection?



Estimates from 2 to 29 TW radiogenic power in the mantle

Earth's energy budget

Total heat loss 46±3 TW



radiogenic + primordial heat + other...

U Th K

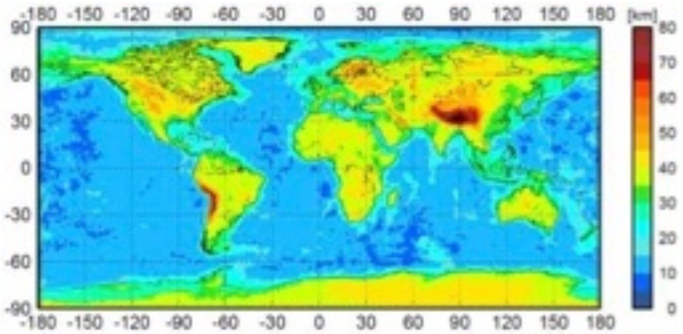
Composition of Silicate Earth (BSE)

- **“Geochemical”** estimate
  - Ratios of RLE abundances constrained by C1 chondrites
  - Absolute abundances inferred from Earth rock samples
  - *McDonough & Sun (1995), Allègre (1995), Hart & Zindler (1986), Palme & O’Neill (2003),* ***Arevalo et al. (2009)***
- **“Cosmochemical”** estimate
  - Isotopic similarity between Earth rocks and E-chondrides
  - Build the Earth from E-chondrite material
  - ***Javoy et al. (2010)***
  - also “collisional erosion” models (*O’Neill & Palme 2008*)
- **“Geodynamical”** estimate
  - Based on a classical parameterized convection model
  - Requires a high mantle Urey ratio, i.e., high U, Th, K

TW radiogenic power

BSE	Mantle
20±4	**13±4**
11±2	**4±2**
33±3	**26±3**

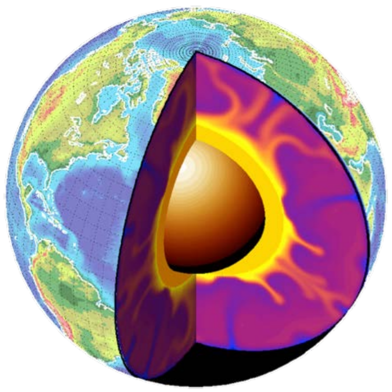
BSE = Mantle + Crust



Oceanic: 0.22 ± 0.03 TW

Continental: 6.8 (+1.4/–1.1) TW

?



Approach:

Use noble gas isotopic ratios
from gases originating at depth

- Why now?
- How to calculate ^{39}Ar production rate
- Some results

Isotopes of Argon

34 known isotopes

^{40}Ar … radiogenic, stable

^{39}Ar … cosmo/nucleogenic, $t_{1/2} = 269$ y

^{36}Ar … primordial, stable

Atmosphere

^{40}Ar from degassing of Earth over 4.5 Gy

^{39}Ar produced cosmogenically from ^{40}Ar

$^{40}\mathrm{Ar}/^{36}\mathrm{Ar} = 295$

$^{39}\mathrm{Ar}/^{40}\mathrm{Ar} = 8\times10^{-16}$

Underground

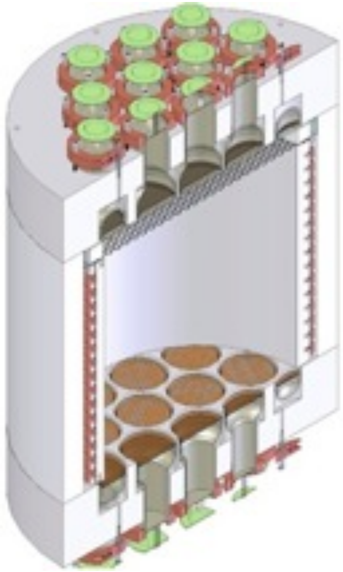
^{40}Ar produced by electron capture on ^{40}K

^{39}Ar produced nucleogenically from ^{39}K

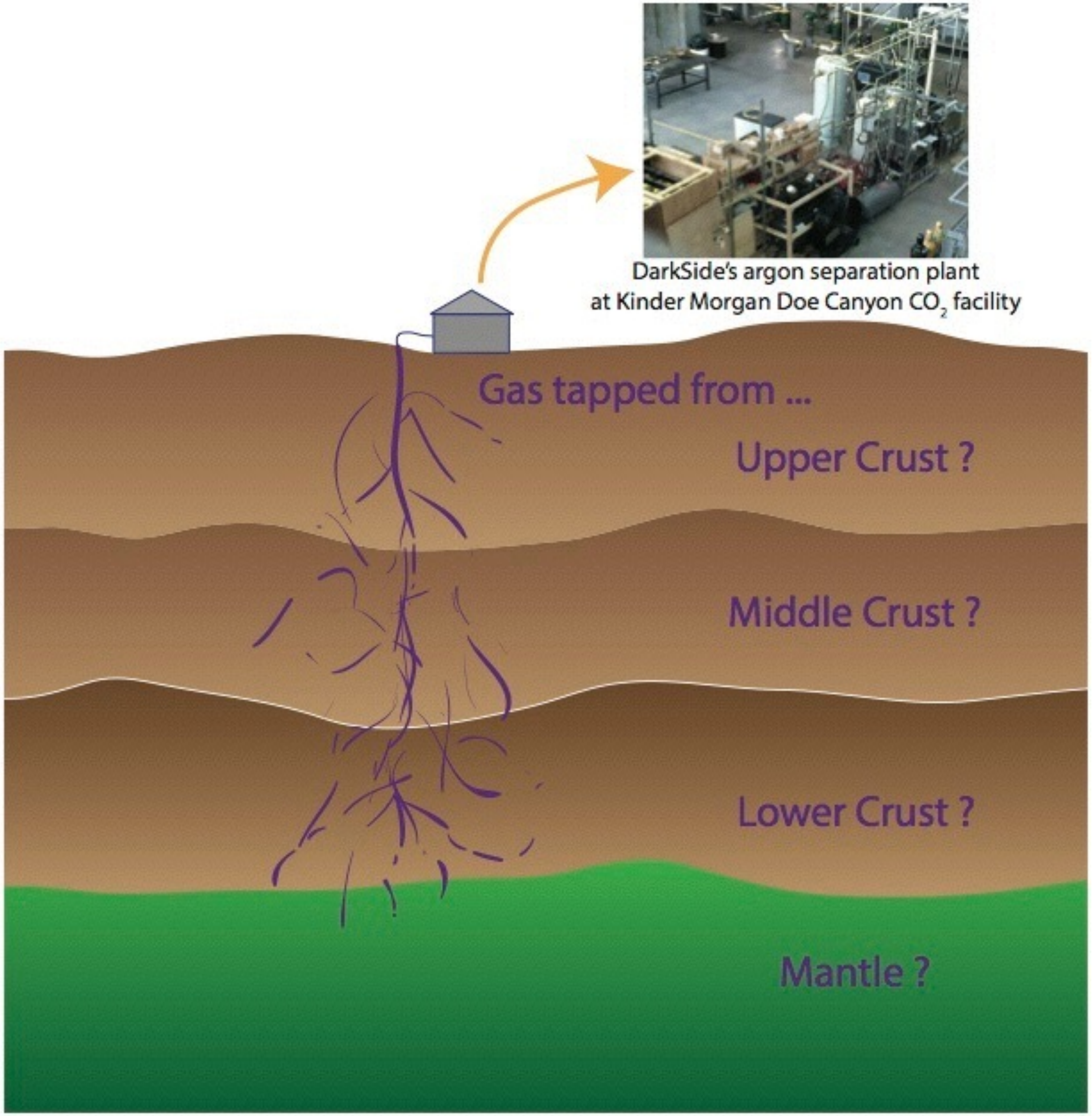
$^{39}\mathrm{Ar}/^{40}\mathrm{Ar} < 0.006$ atmospheric

Dark matter WIMP search

- Dark matter detectors looking for Weakly Interacting Massive Particles (WIMPs) require low radioactivity argon



- Atmospheric level ($^{39}Ar/^{40}Ar=8\times10^{-16}$) is too high
- Gas from deep CO_2 wells shows lower level of ^{39}Ar (e.g., Cortez CO, Bueyeros NM)
- $^{39}Ar/^{40}Ar$ – challenging measurements…
  – low-level radioactive decay counting
  – Atomic Trap Trace Analysis (ATTA)



DarkSide's argon separation plant
at Kinder Morgan Doe Canyon CO_2 facility

Gas tapped from ...

Upper Crust ?

Middle Crust ?

Lower Crust ?

Mantle ?

Nuclear physics notation:

A(a,b)B

$A + a \rightarrow b + B$

A … target nuclide
a … projectile
b … ejectile
B … product nuclide

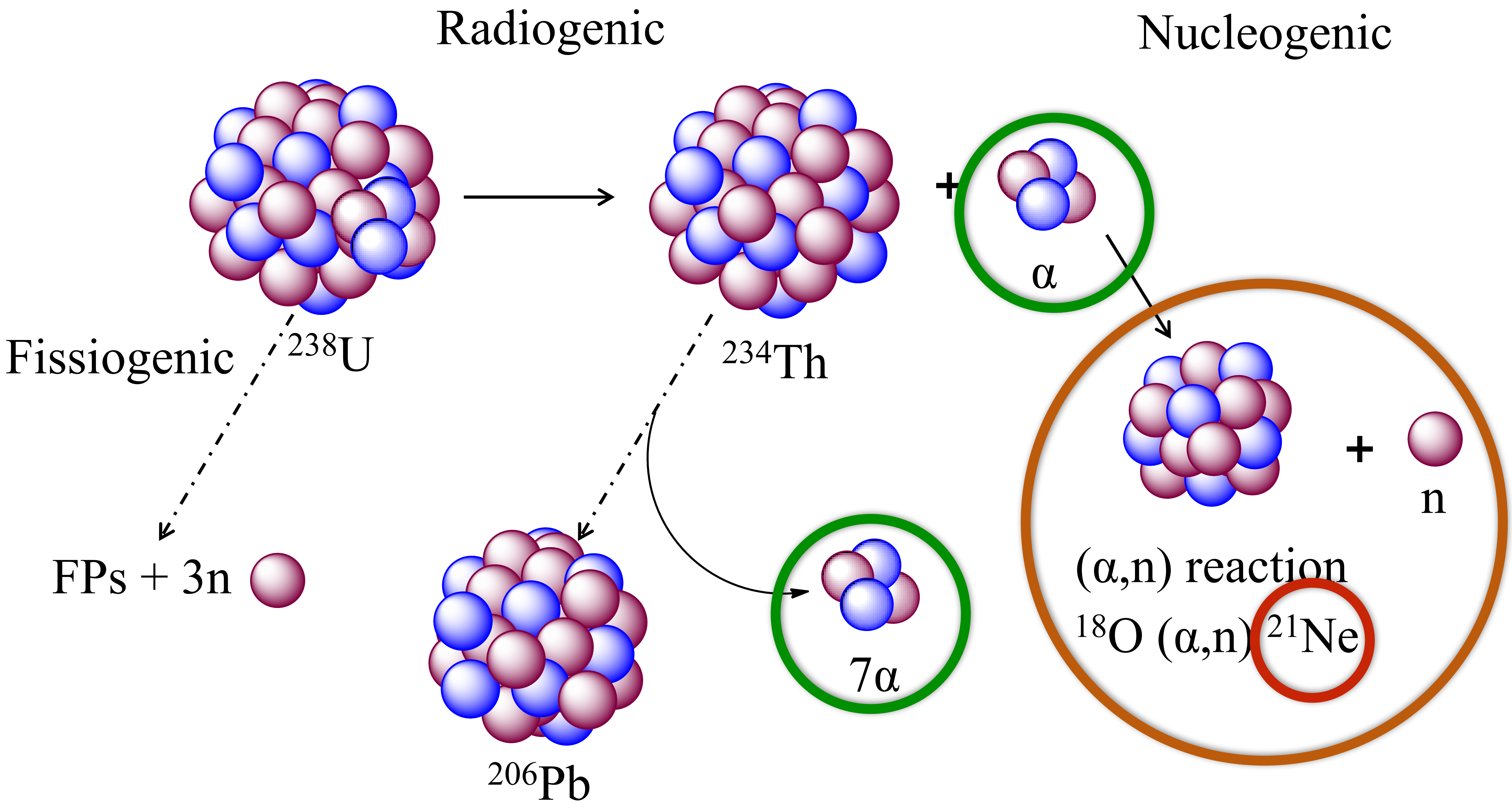
(α,n)
(n,p)
(n,a)
(n,2n)
…

$^{40}\mathrm{Ar}(n,2n)^{39}\mathrm{Ar}$
atmosphere, cosmogenic

Nucleogenic production

- Decay of radioactive U and Th in Earth's interior produce α particles
- (α, n) reactions on light isotopes produce neutrons
- Neutrons are also produced by spontaneous fission of U
- (n,p) reaction then produces ^{39}Ar from ^{39}K
- ⇒ Measurement of isotopic ratios in outgassing rock can inform us about the U, Th, K

1. U, Th decay produces α's



Radiogenic

Nucleogenic

Fissiogenic

^{238}U

^{234}Th

+

α

FPs + 3n

^{206}Pb

7α

+

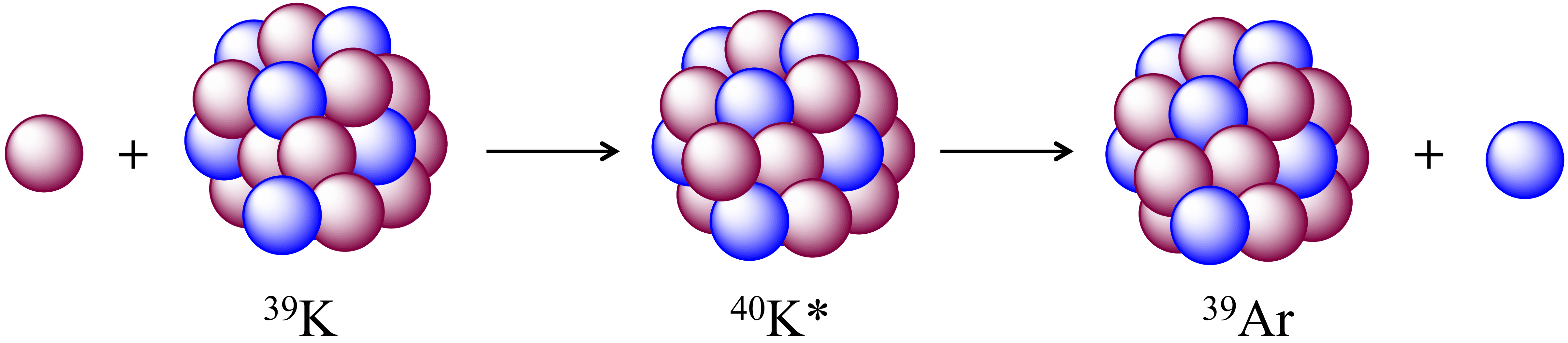
n

(α,n) reaction

^{18}O (α,n) ^{21}Ne

2. (α,n) produce neutrons

^{39}K(n,p) produces ^{39}Ar



^{39}K

^{40}K*

^{39}Ar

composite
nucleus

Noble gas isotopic ratios

- ^{21}Ne production rate proportional to [U+Th]
- ^{39}Ar production rate proportional to [K] × [U+Th]
- ^{40}Ar production rate proportional to [K]

therefore

- ^{39}Ar/^{40}Ar proportional to [U+Th]
- ^{39}Ar/^{21}Ne proportional to [K]
- ^{40}Ar/^{21}Ne proportional to [K]/[U+Th]

Calculating ^{39}Ar nucleogenic production rate

- α emission from natural radionuclides
- neutron production by α-induced reactions
- ^{39}K(n,p)^{39}Ar

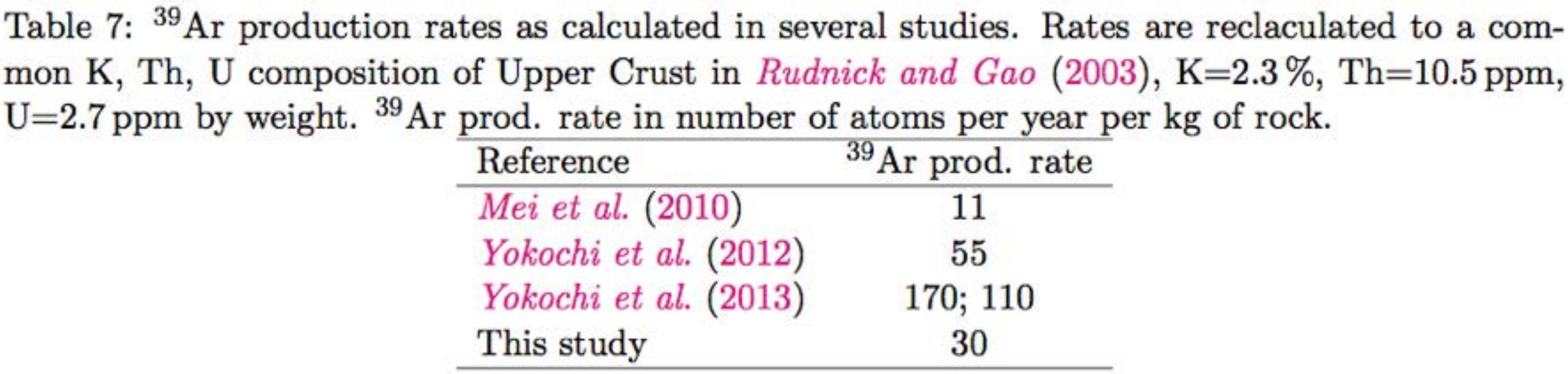
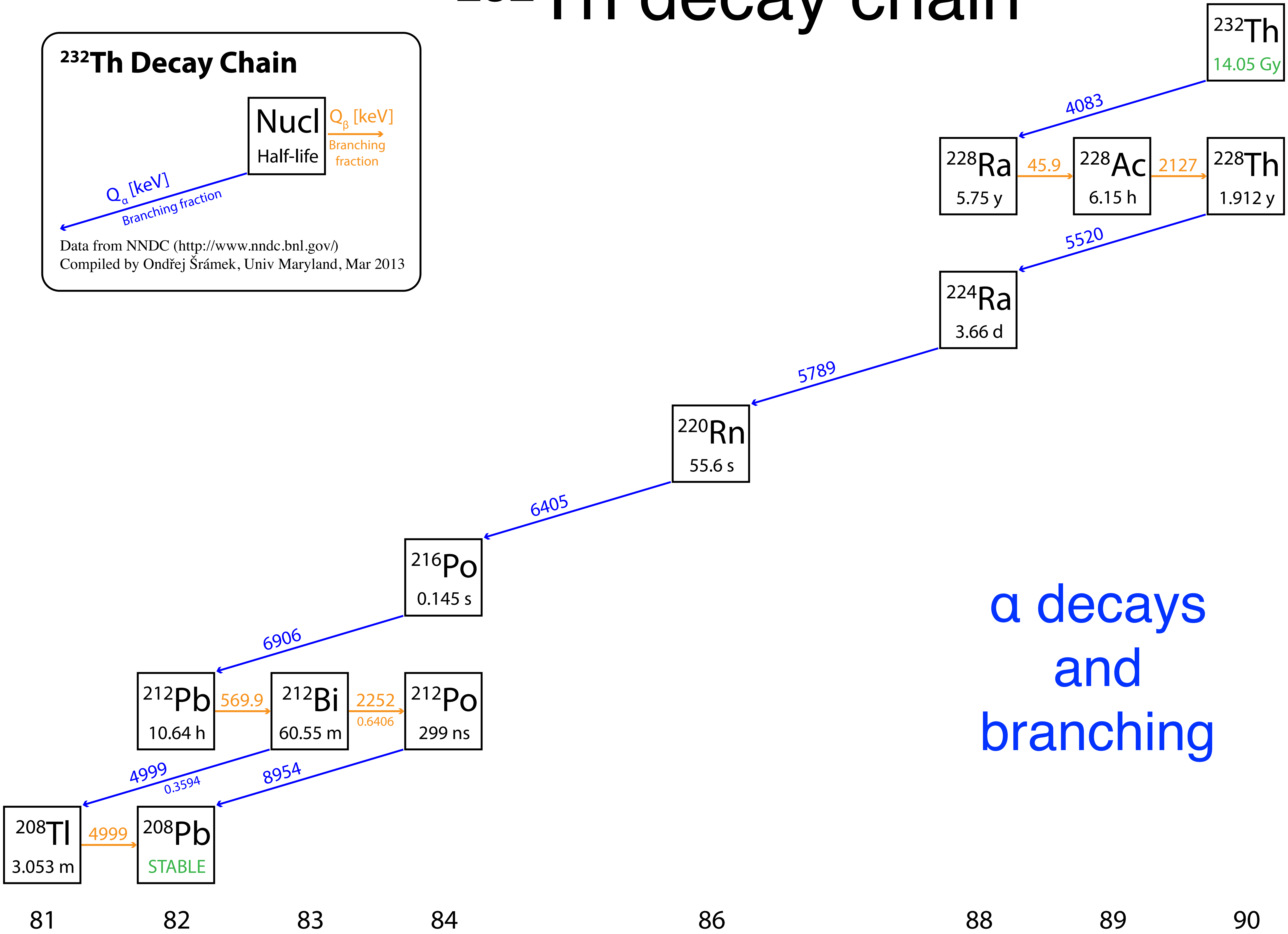


Table 7: ^{39}Ar production rates as calculated in several studies. Rates are reclaculated to a common K, Th, U composition of Upper Crust in *Rudnick and Gao* (2003), K=2.3 %, Th=10.5 ppm, U=2.7 ppm by weight. ^{39}Ar prod. rate in number of atoms per year per kg of rock.

Reference	^{39}Ar prod. rate
Mei et al. (2010)	11
Yokochi et al. (2012)	55
Yokochi et al. (2013)	170; 110
This study	30

^{232}Th decay chain

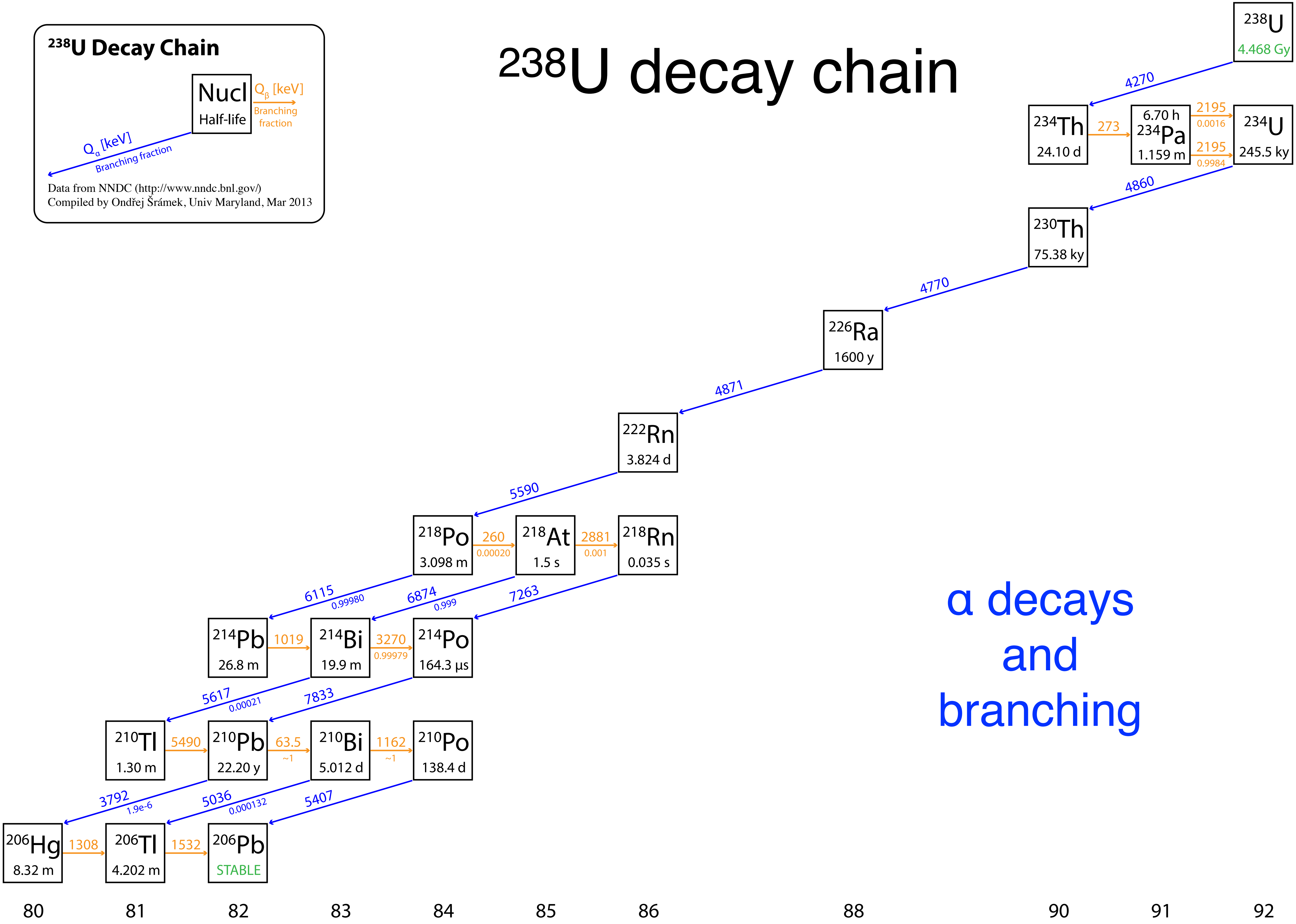


Data from NNDC (http://www.nndc.bnl.gov/)
Compiled by Ondřej Šrámek, Univ Maryland, Mar 2013

α decays
and
branching

data from National Nuclear Data Center, http://www.nndc.bnl.gov/

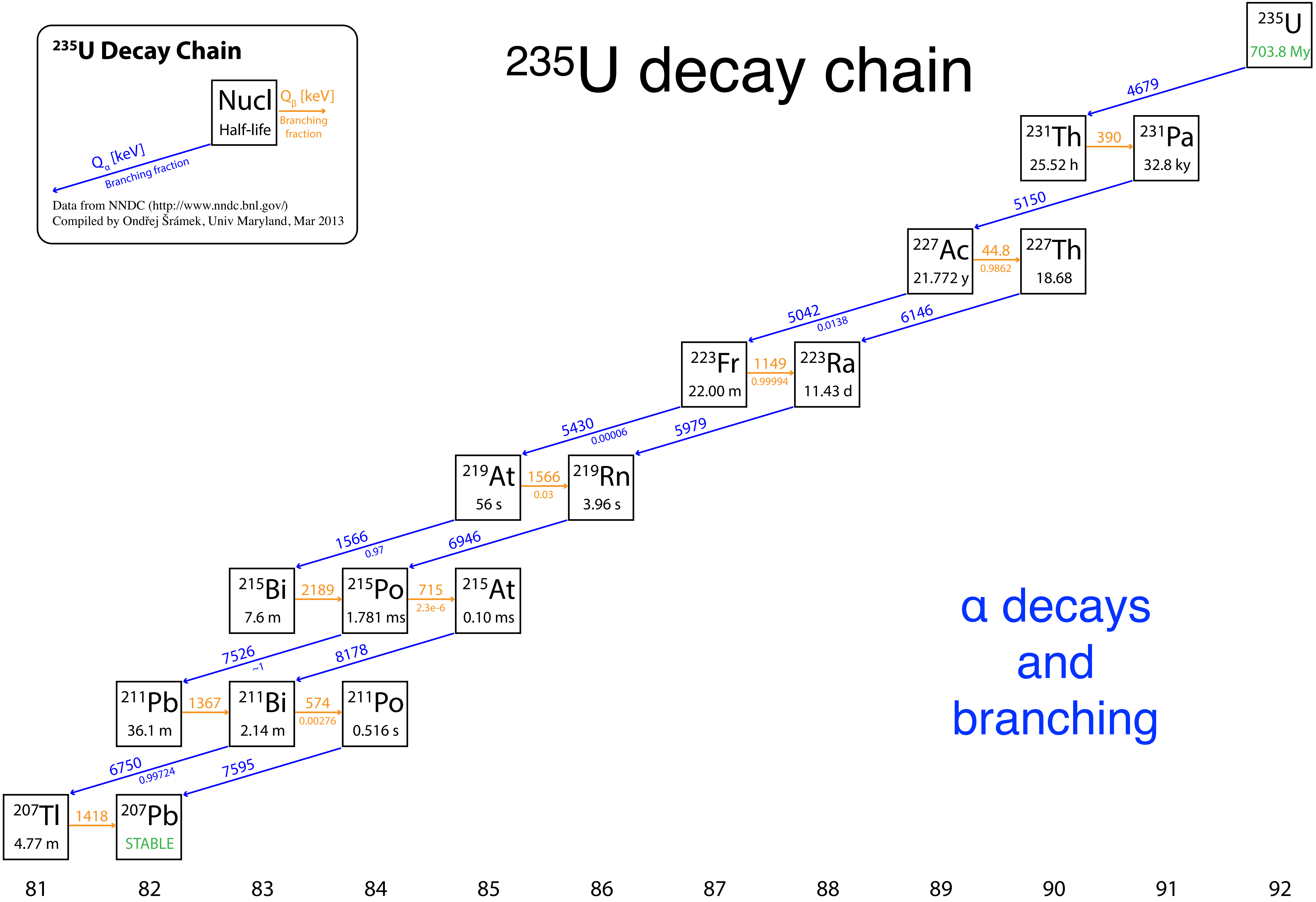
^{238}U decay chain



α decays
and
branching

data from National Nuclear Data Center, http://www.nndc.bnl.gov/

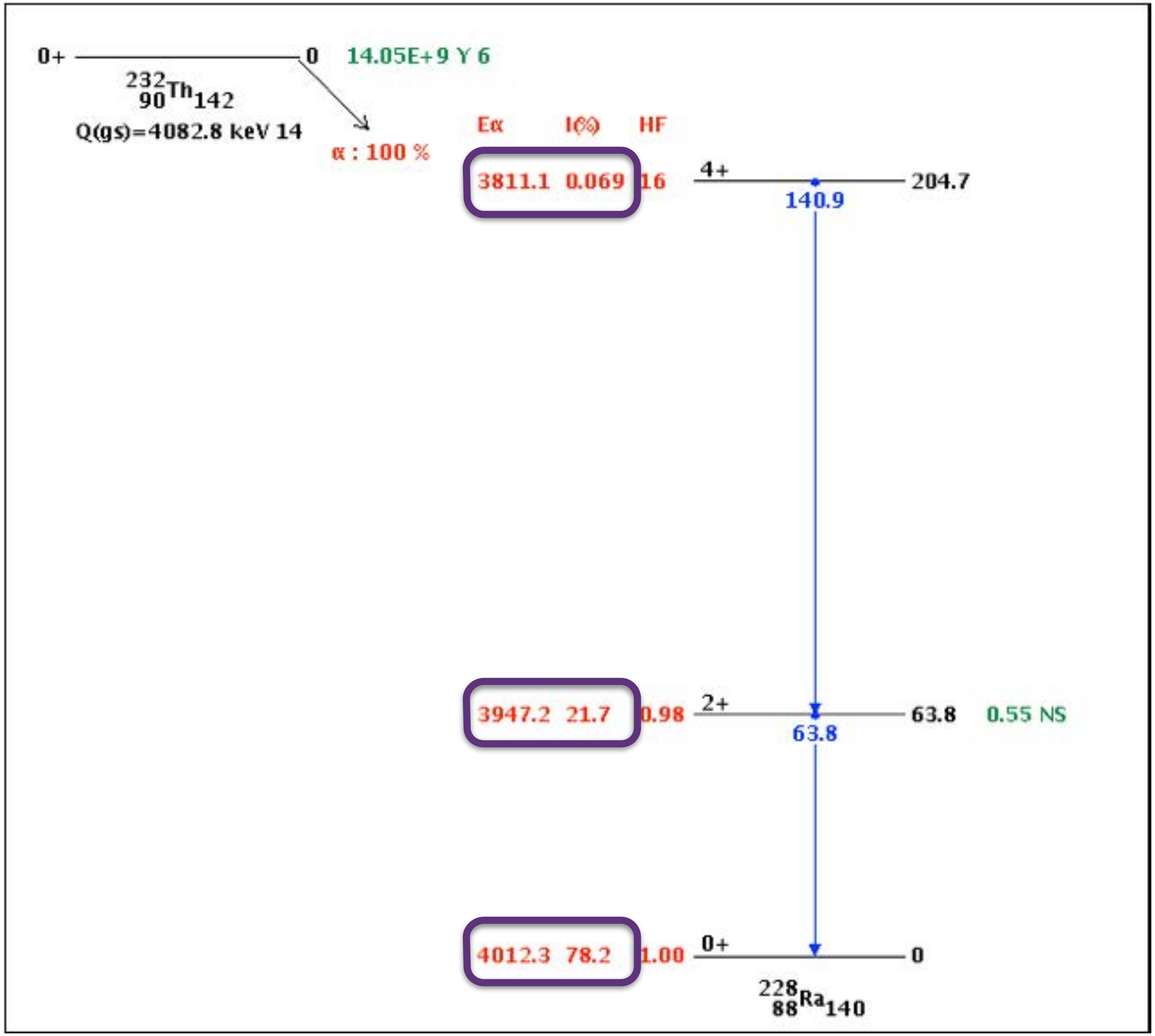
^{235}U decay chain



α decays
and
branching

data from National Nuclear Data Center, http://www.nndc.bnl.gov/

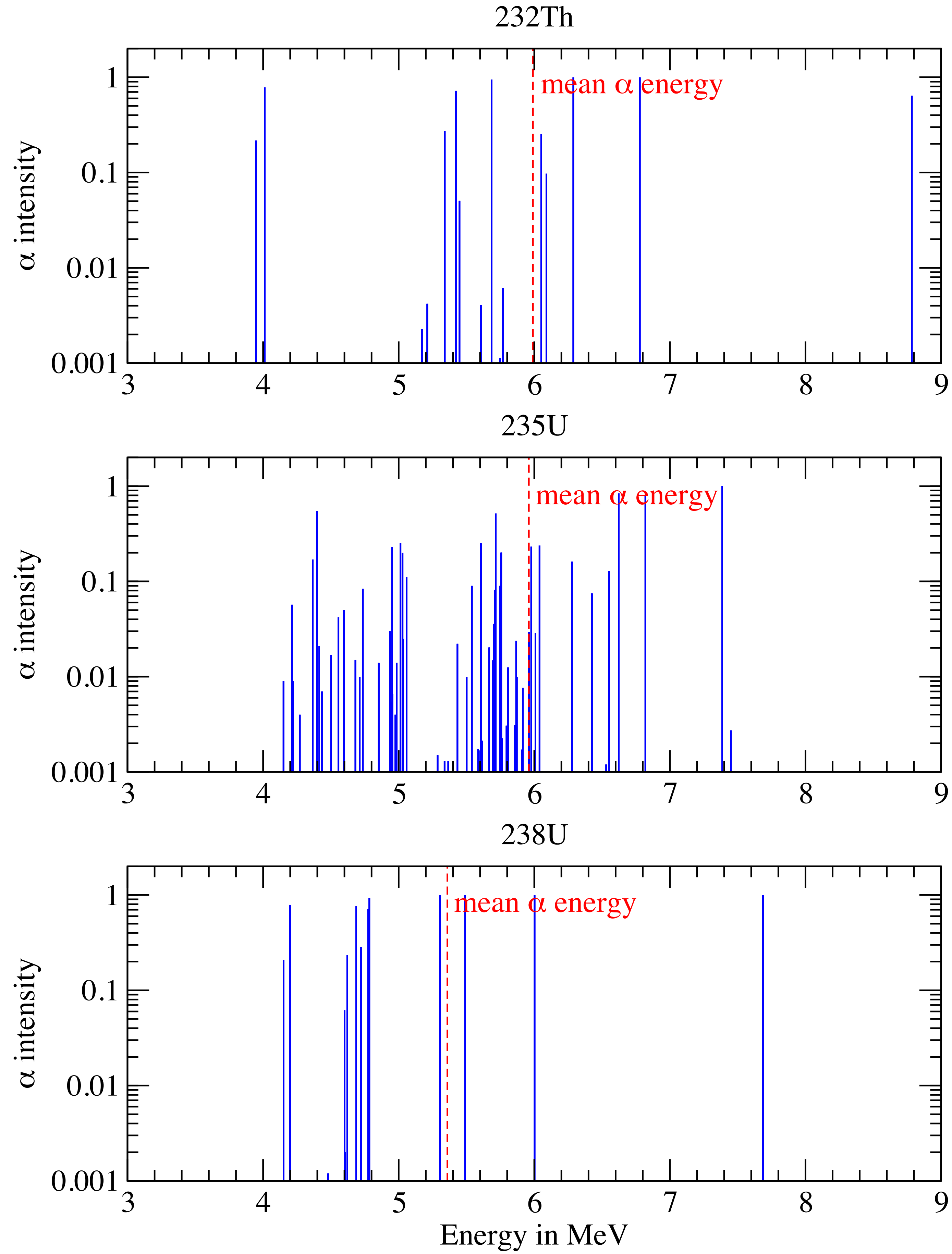
^{232}Th α decay scheme



α energies and intensities

data from National Nuclear Data Center, http://www.nndc.bnl.gov/

Natural alpha emission energy spectra



α's/decay:

6

7

8

Calculating ^{39}Ar nucleogenic production rate

- α emission from natural radionuclides
- neutron production by α-induced reactions
- $^{39}K(n,p)^{39}Ar$

(α,n) neutron production and spectrum

- α emitted at initial energy $E_{\alpha 0}$
- α slows down and eventually stops (E=0) in the rock
- before it stops, it can participate in (α,n) reaction

neutron production function

neutrons per 1 α particle

cross section

$$P_i(E_{\alpha_0}) = N_i \int_0^{E_{\alpha_0}} \frac{\sigma^i_{\alpha,n}(E_\alpha)}{\left(-\frac{\mathrm{d}E_\alpha}{\mathrm{d}x}\right)} \mathrm{d}E_\alpha$$

atomic density

stopping power

neutron spectrum

spectrum (or differential c.s.)

$$\frac{\mathrm{d}P_i}{\mathrm{d}E_n}(E_{\alpha_0}, E_n) = N_i \int_0^{E_{\alpha_0}} \frac{\frac{\mathrm{d}\sigma^i_{\alpha,n}}{\mathrm{d}E_n}(E_\alpha, E_n)}{\left(-\frac{\mathrm{d}E_\alpha}{\mathrm{d}x}\right)} \mathrm{d}E_\alpha$$

(α,n) neutron yield and production rate

neutron production function

neutrons per 1 α particle

cross section

$$P_i(E_{\alpha_0}) = N_i \int_0^{E_{\alpha_0}} \frac{\sigma^i_{\alpha,n}(E_\alpha)}{\left(-\frac{\mathrm{d}E_\alpha}{\mathrm{d}x}\right)} \mathrm{d}E_\alpha$$

atomic density

stopping power

neutron spectrum

spectrum (or differential c.s.)

$$\frac{\mathrm{d}P_i}{\mathrm{d}E_n}(E_{\alpha_0}, E_n) = N_i \int_0^{E_{\alpha_0}} \frac{\frac{\mathrm{d}\sigma^i_{\alpha,n}}{\mathrm{d}E_n}(E_\alpha, E_n)}{\left(-\frac{\mathrm{d}E_\alpha}{\mathrm{d}x}\right)} \mathrm{d}E_\alpha$$

neutron yield

neutrons per decay of 1 atom of parent nuclide

α decays

E levels

targets

$$Y_{(\alpha,n)} = \sum_{k=1}^{K} b_k \sum_{l=1}^{L_k} f_l^\alpha \sum_{i=1}^{I} P_i(E_l)$$

branching ratio

level intensity

neutron production rate

neutrons per unit time per unit mass of rock

elem. abundance

nat.isot.rat.

$$S_n = \lambda \frac{AXN_A}{M} Y$$

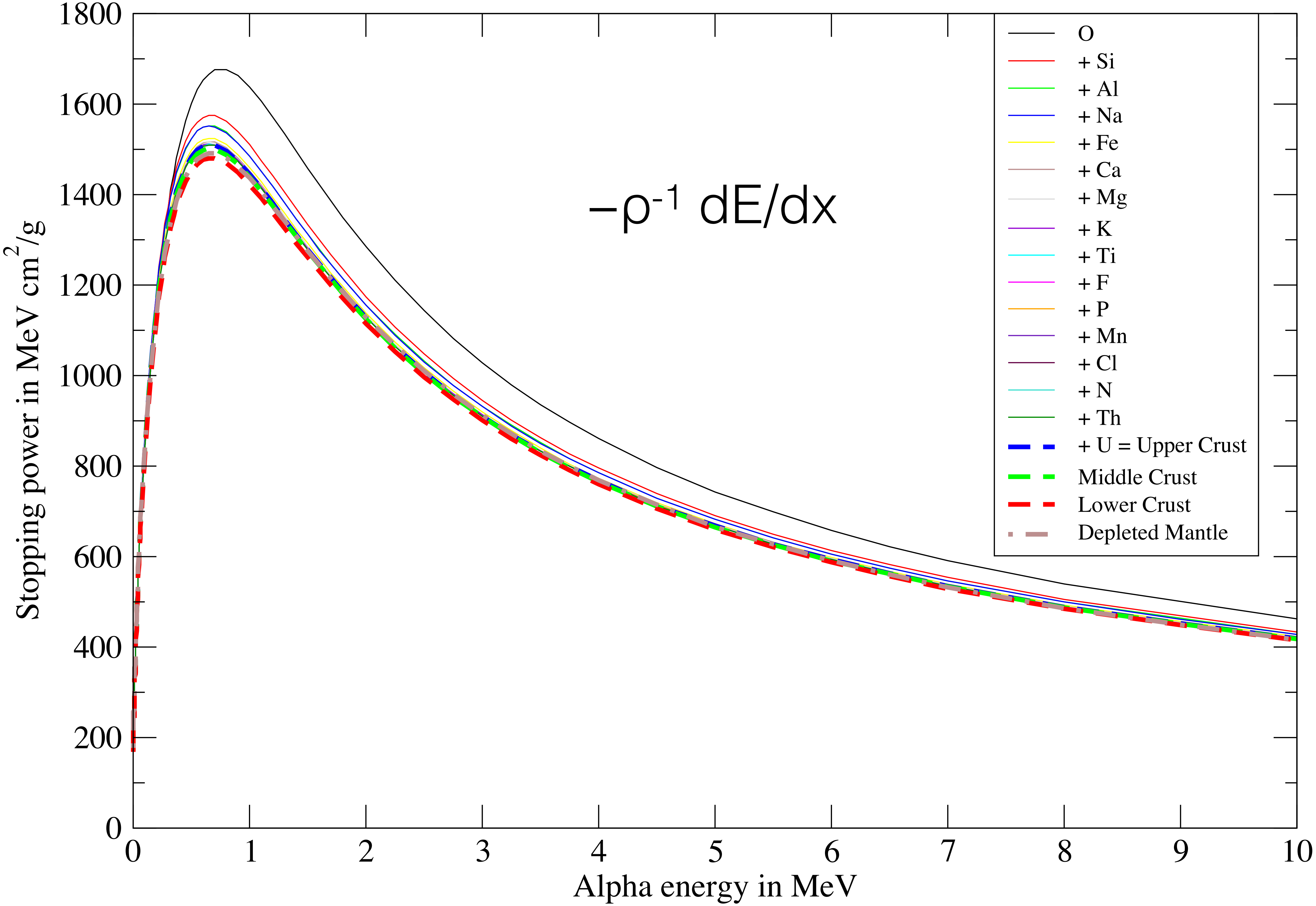
decay constant

atomic mass

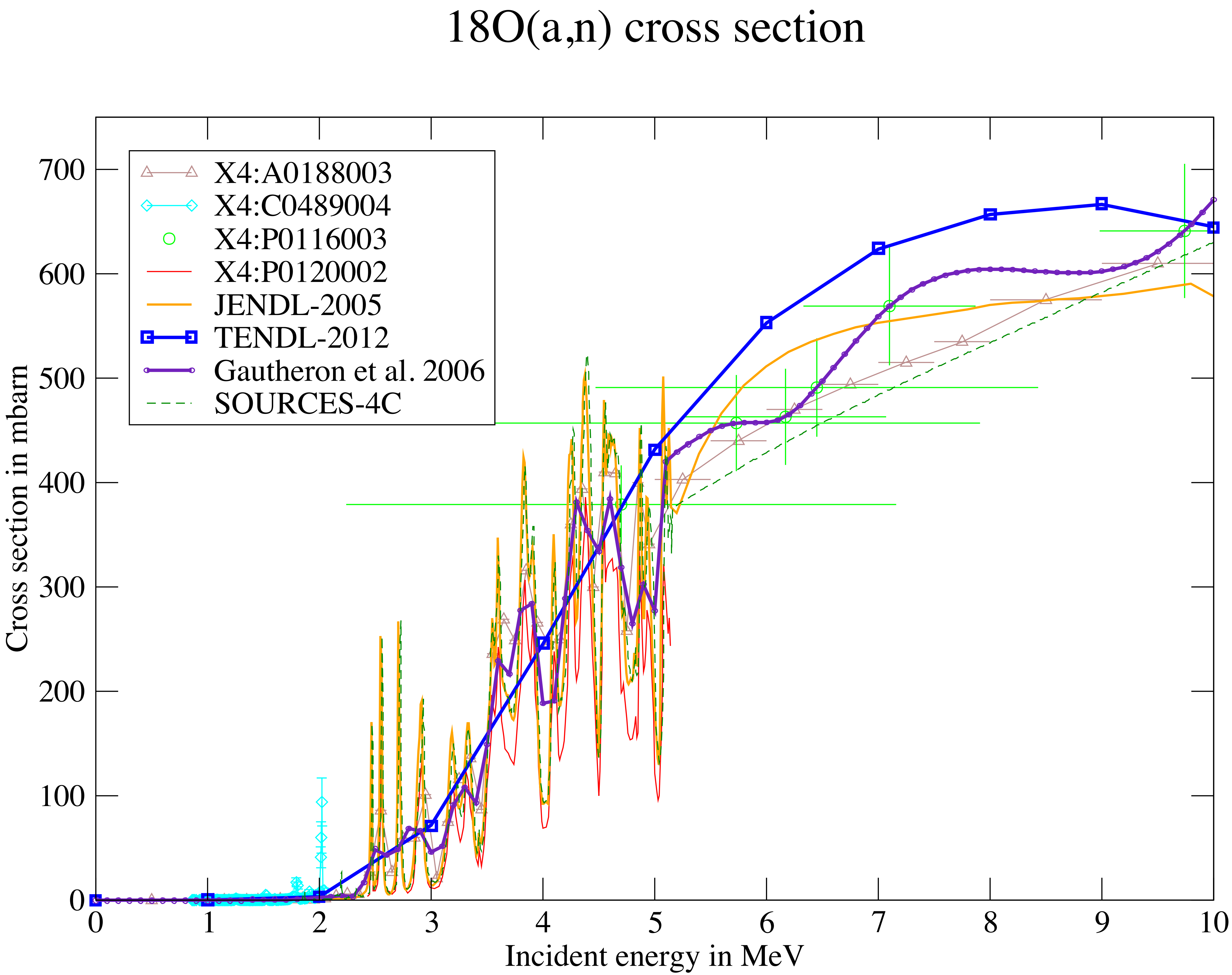
inputs…

Stopping power of alphas in rock

SRIM calc, RG03 / SS04 composition and CRUST2.0 / PREM density (2.70 - 2.88 - 3.05 / 3.42 g/cm^3)

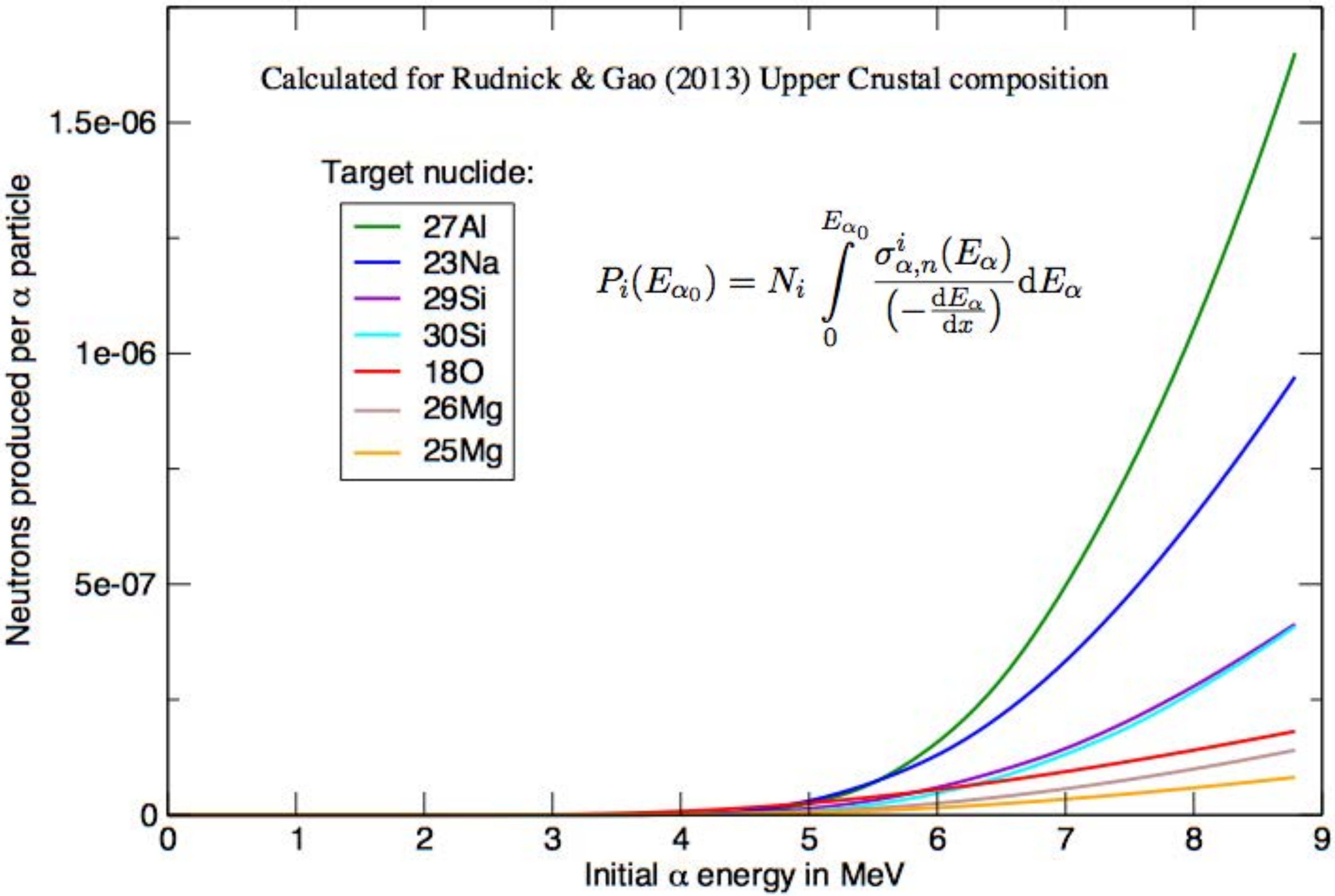


data from Stopping and Range of Ion in Matter, http://srim.org/



We use: cross sections calculated by TALYS code, http://www.talys.eu/

Neutron production function



Calculating neutron spectra

1. Non-relativistic reaction kinematics

Ground state-to-ground state

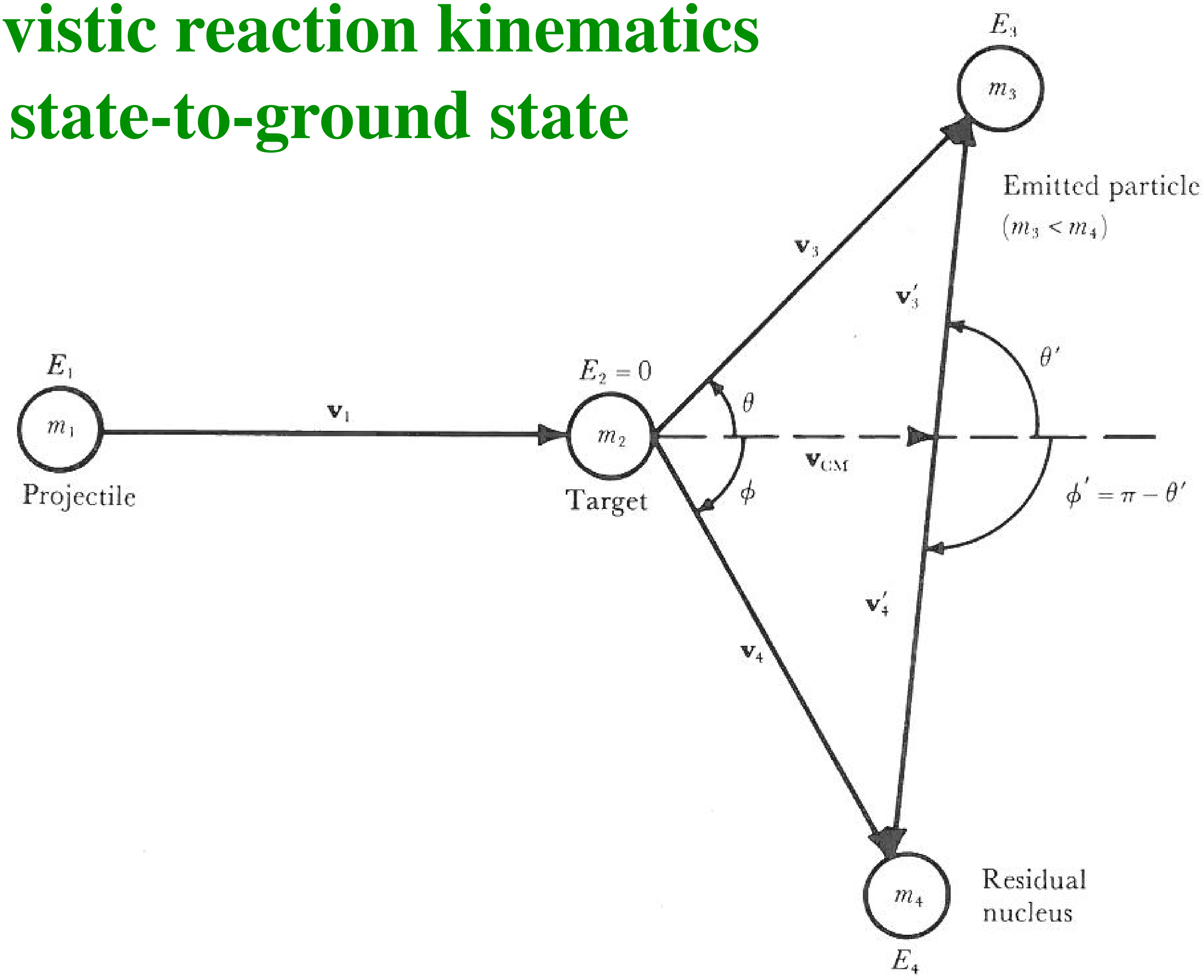
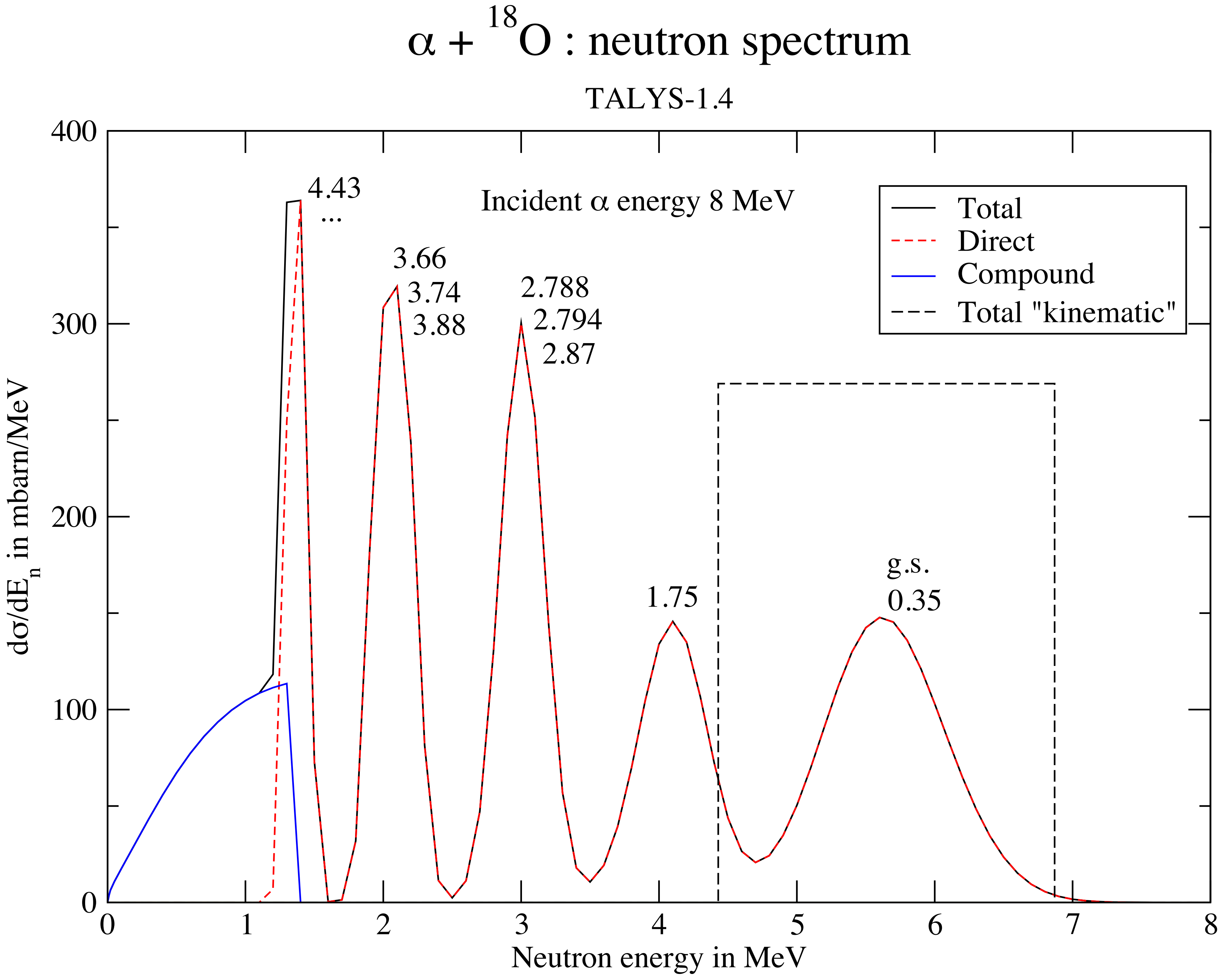


Fig. C-4. Vector diagram showing the relationship of kinematic quantities in the reaction process $m_1 + m_2 \rightarrow m_3 + m_4$.

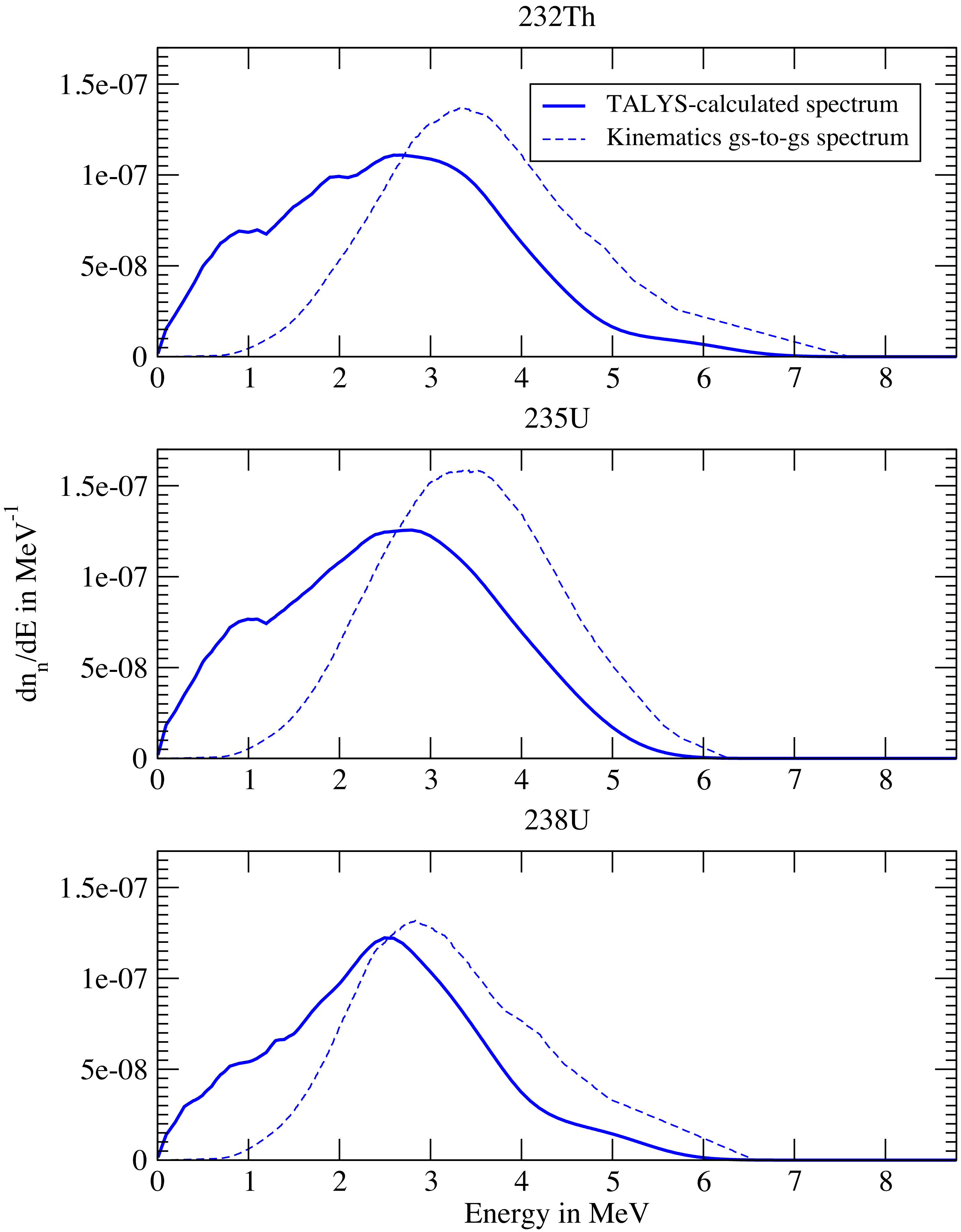
2. More complete physical picture: TALYS code

Neutron spectrum for 8 MeV α + ^{18}O



We use: spectra calculated by TALYS code, http://www.talys.eu/

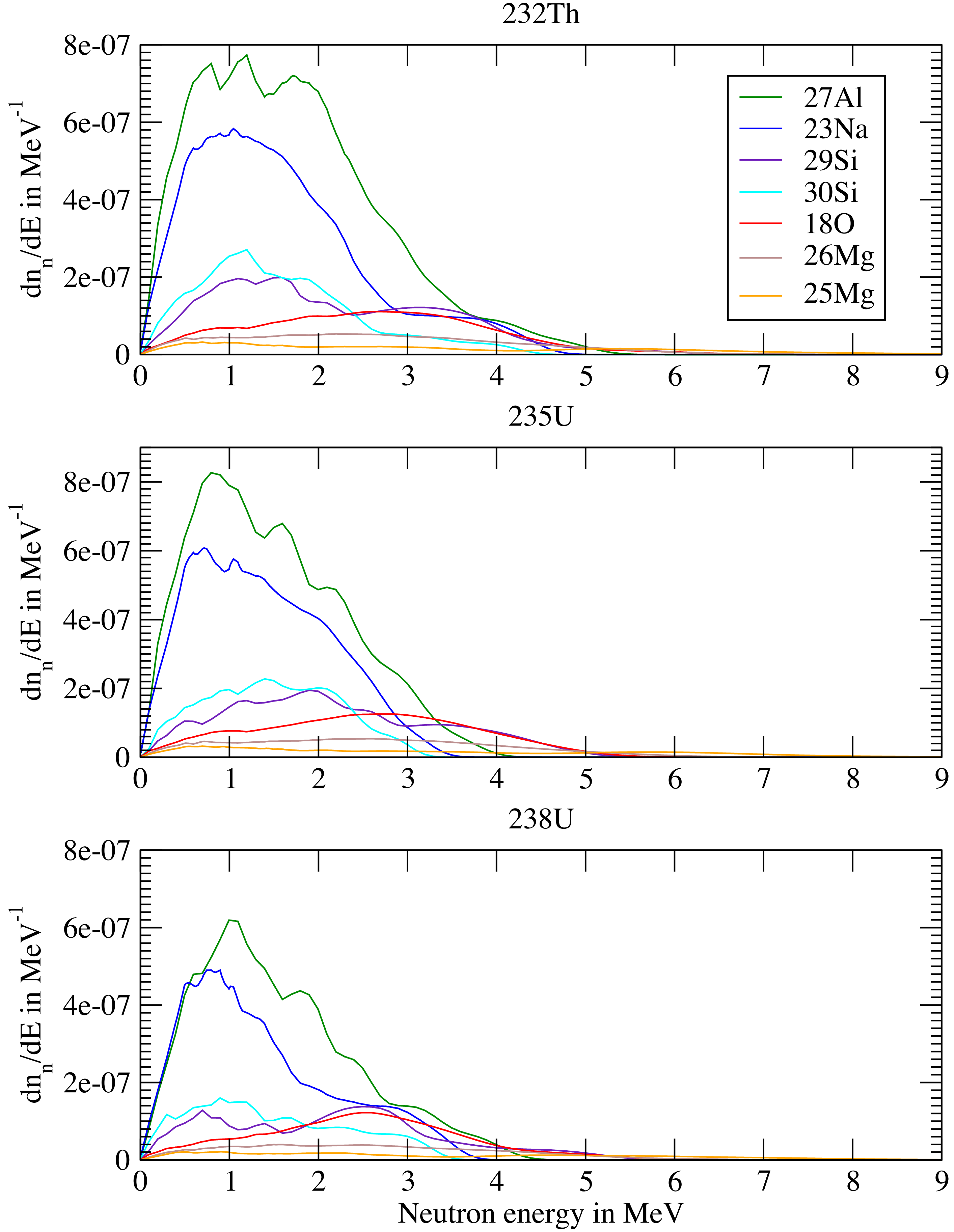
$\alpha + {}^{18}O$: neutron energy spectra



$$\frac{\mathrm{d}P_i}{\mathrm{d}E_n}(E_{\alpha_0}, E_n) = N_i \int_0^{E_{\alpha_0}} \frac{\frac{\mathrm{d}\sigma^i_{\alpha,n}}{\mathrm{d}E_n}(E_\alpha, E_n)}{\left(-\frac{\mathrm{d}E_\alpha}{\mathrm{d}x}\right)} \mathrm{d}E_\alpha$$

+ sum up over all α-decays,
all α levels

α + target : neutron energy spectra [TALYS]



$$\frac{\mathrm{d}P_i}{\mathrm{d}E_n}(E_{\alpha_0},E_n) = N_i \int_0^{E_{\alpha_0}} \frac{\frac{\mathrm{d}\sigma^i_{\alpha,n}}{\mathrm{d}E_n}(E_\alpha,E_n)}{\left(-\frac{\mathrm{d}E_\alpha}{\mathrm{d}x}\right)} \mathrm{d}E_\alpha$$

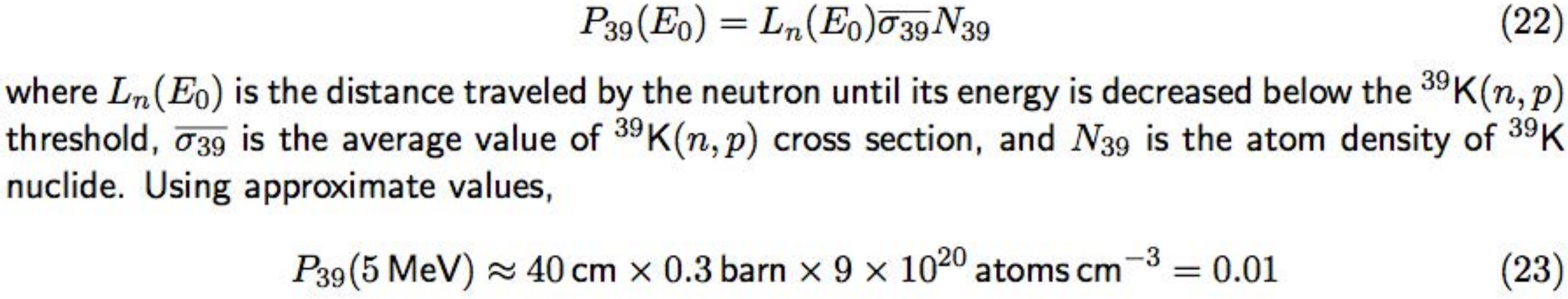
+ sum up over all α-decays,
all α levels

Calculating ^{39}Ar nucleogenic production rate

- α emission from natural radionuclides
- neutron production by α-induced reactions
- ^{39}K(n,p)^{39}Ar, also ^{24}Mg(n,α)^{21}Ne

Neutrons propagating and interacting in the rock

- Competition between neutron scattering, various neutron-induced reactions on various targets
- We are interested in specific reactions
- Back-of-the-envelope calculations give us an order of magnitude answer:



$$P_{39}(E_0) = L_n(E_0)\overline{\sigma_{39}}N_{39} \tag{22}$$

where $L_n(E_0)$ is the distance traveled by the neutron until its energy is decreased below the $^{39}\mathrm{K}(n,p)$ threshold, $\overline{\sigma_{39}}$ is the average value of $^{39}\mathrm{K}(n,p)$ cross section, and N_{39} is the atom density of $^{39}\mathrm{K}$ nuclide. Using approximate values,

$$P_{39}(5\,\mathrm{MeV}) \approx 40\,\mathrm{cm} \times 0.3\,\mathrm{barn} \times 9 \times 10^{20}\,\mathrm{atoms\,cm^{-3}} = 0.01 \tag{23}$$

- We use MCNP6 code for a more educated calculation (Monte Carlo N-Particle, http://mcnp.lanl.gov)

Results

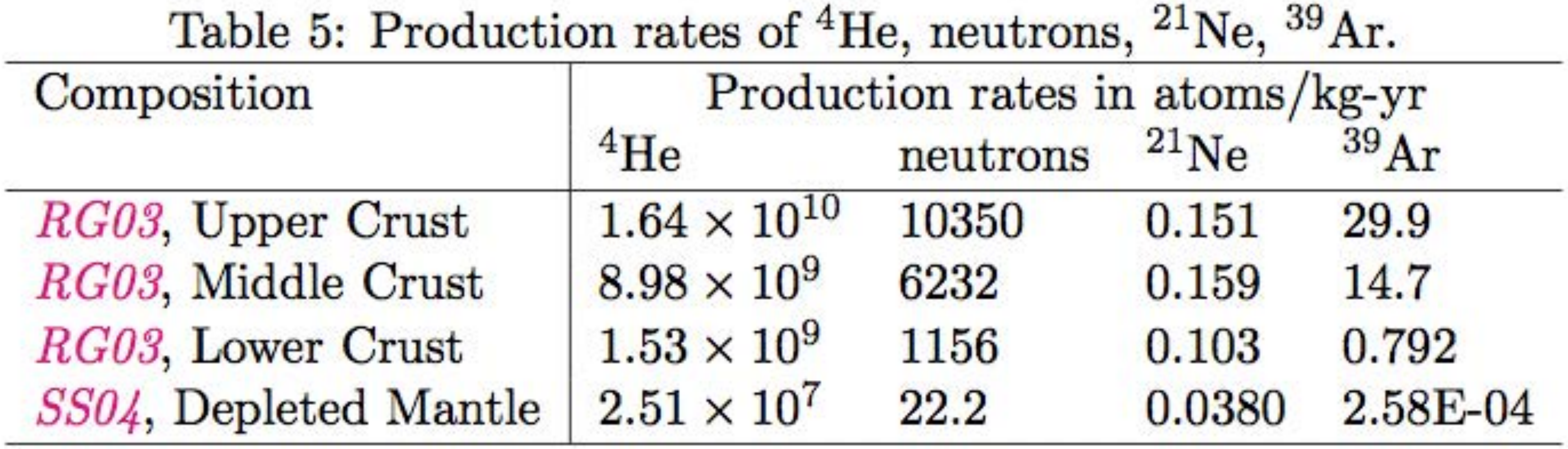


Table 5: Production rates of ^{4}He, neutrons, ^{21}Ne, ^{39}Ar.

Composition	Production rates in atoms/kg-yr			
	^{4}He	neutrons	^{21}Ne	^{39}Ar
RG03, Upper Crust	1.64×10^{10}	10350	0.151	29.9
RG03, Middle Crust	8.98×10^{9}	6232	0.159	14.7
RG03, Lower Crust	1.53×10^{9}	1156	0.103	0.792
SS04, Depleted Mantle	2.51×10^{7}	22.2	0.0380	2.58E-04

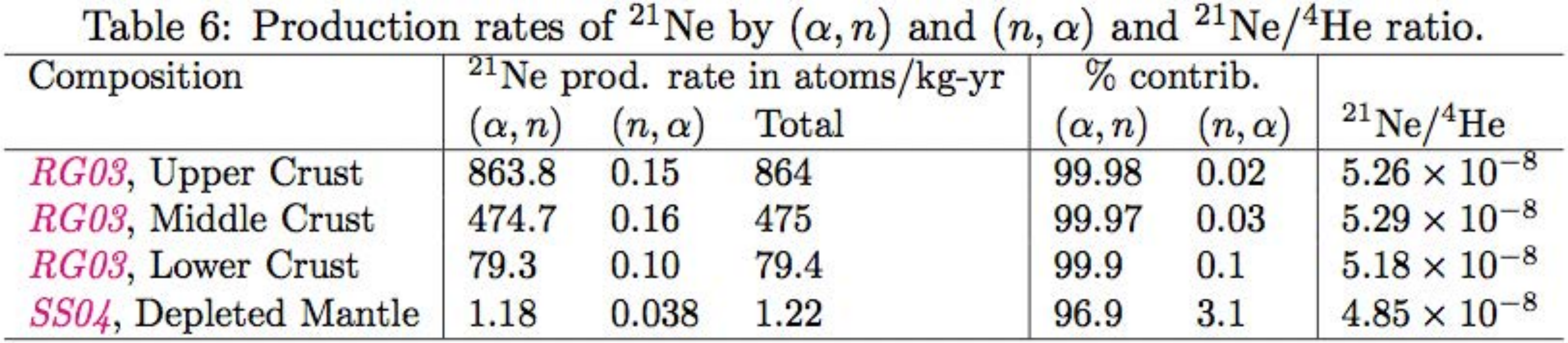


Table 6: Production rates of ^{21}Ne by (α, n) and (n, α) and ^{21}Ne/^{4}He ratio.

Composition	^{21}Ne prod. rate in atoms/kg-yr			% contrib.		
	(α, n)	(n, α)	Total	(α, n)	(n, α)	^{21}Ne/^{4}He
RG03, Upper Crust	863.8	0.15	864	99.98	0.02	5.26×10^{-8}
RG03, Middle Crust	474.7	0.16	475	99.97	0.03	5.29×10^{-8}
RG03, Lower Crust	79.3	0.10	79.4	99.9	0.1	5.18×10^{-8}
SS04, Depleted Mantle	1.18	0.038	1.22	96.9	3.1	4.85×10^{-8}

Yokochi et al. (1997): ^{21}Ne/^{4}He = 4.5×10^{-8}

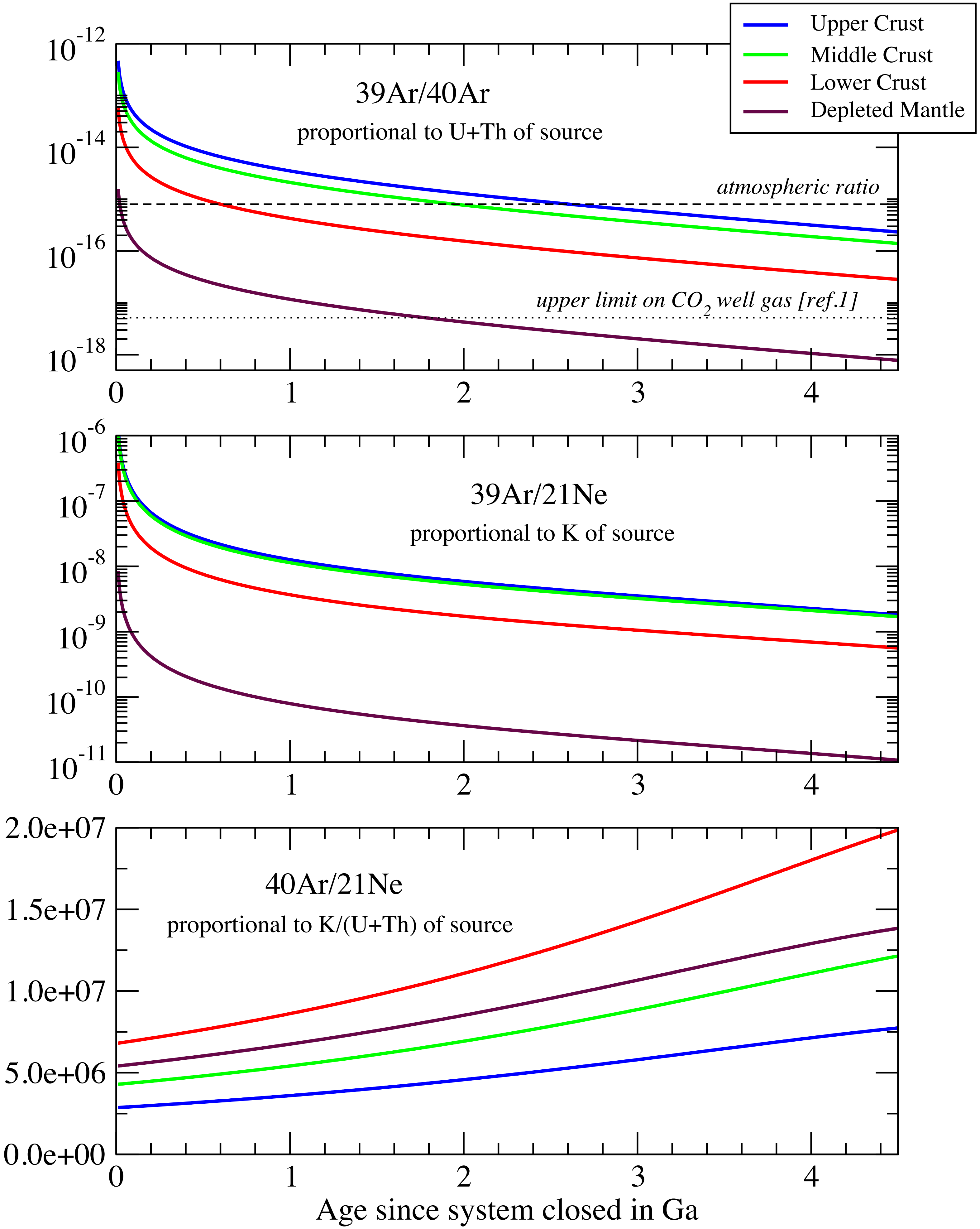
Isotopic ratios

Trade-off between composition and “age” of system

Closed system:

^{21}Ne, ^{40}Ar accumulate

^{39}Ar steady-state level



Summary

- New calculations of nucleonic production rates
- Combination of state-of-the-art nuclear physics tools (TALYS, MCNP6) and my own code to put everything together
- (Re-)Learned aspects of nuclear physics
- Results of interest to hydrology, dark matter experiments, crustal & mantle geochemistry
- We expect the ^{39}Ar detection methods to improve