



## TENDL-2017: THE MAKING OF MULTI-FACETED TECHNOLOGICAL NUCLEAR DATA LIBRARY

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Multi-purpose methodical nuclear data libraries generated by TALYS/T6 as Evaluated Nuclear Data Library TENDL have been released annually since 2008. Considerable experience has been acquired during those early production of such unique, truly multi-faceted, multi-particle nuclear data libraries based on the feedback from the developers, evaluators, processing experts and, most importantly, users. The backbone of this achievement is simple and robust: completeness, quality, upgradability and, most of all, reproducibility and methodology. Since TENDL has been seamlessly adopted by many different applications (accelerator, astrophysics, fusion, fission, medical) that require multi-faceted nuclear reaction data forms for shielding, radio-protection, transmutation, materials or earth sciences, it is felt necessary to understand its strengths and remaining weaknesses. The essential knowledge is not the TENDL library itself, but rather the necessary methods, processes, codes, tools and know-how that go into the making of every evaluations of such a library. Current efforts are focused on a proper evaluation of the underlying physics and incorporation of information and metrics into the scientific TALYS/T6 system.

### I. INTRODUCTION

Industry recognized continental legacy nuclear data libraries (ENDF/B in the USA; JENDL in Japan; JEFF for the OECD/NEA Databank member country, CENDL for China, ROSFOND for Russia) are assembled over decades by hand: evaluators have added nuclides/reactions/energies as and when it was deemed necessary for principally fission applications. The methodology is robust where high-quality, differential or integral, experiments have been performed, but relative to the total set of target nuclides/reactions/energies those libraries are small, targeted to one application and incomplete. They generally do not contain any more than a very small fraction of the nuclear data and observables needed for other non-fission, non-criticality applications. Since many (or most) reactions important for advanced systems (fusion shielding, medical, accelerators, instrumentation and manufacture, security or astrophysics) have little or no experimental differential data, those legacy libraries cannot be relied upon and an alternative is necessary.

The TALYS<sup>1</sup> nuclear models code suite uses various physical models (theoretical and semi-empirical; Optical, Hauser-Feshbach, Exciton, Hartree-fock, Distorted Wave

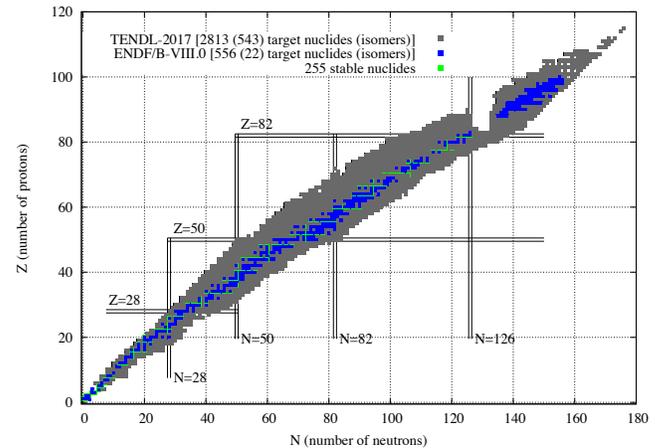


Fig. 1. Nuclear landscape, isotopic targets

Born, Fermi gas, ECIS for the Schrödinger equation, see Fig. 2) to generate and assemble a nuclear data library. TENDL is a nuclear data library covering completely the nuclide/reaction/energy sets, preventing unpolished simulation due to missing or incomplete data sets. As such it can be directly used in both basic physics and novel applications. The 9th version is TENDL-2017<sup>2</sup> which is based on both default and adjusted parameters of the most recent T6 codes: TALYS (nuclear reaction), TAFIS and TANES (fission events), TARES (resonances), TEFAL (ENDF-6 parser) and TASMAN (analytic, statistic), wrapped into a Bayesian Monte-Carlo<sup>3</sup> BMC loop for uncertainty quantification. The TALYS/T6 codes system, combined with a BMC sampling method according to weight of its main nuclear model parameters is uniquely capable of generating the full nuclear data library with complete covariance (model and/or experiment based), enabling thorough nuclear data uncertainty analysis which is not always possible using any other libraries or systems.

### II. NUCLEAR OBSERVABLES FOR SCIENCES AND TECHNOLOGIES

#### II.A. Construction and file assemblage

If it has not been measured, it cannot not exist! Having said that the development of modern nuclear model code, at the request of a user's community that cannot not afford any more gaps in their nuclear data tables, challenge this dogmatism. TALYS/T6 on the contrary follows the rather

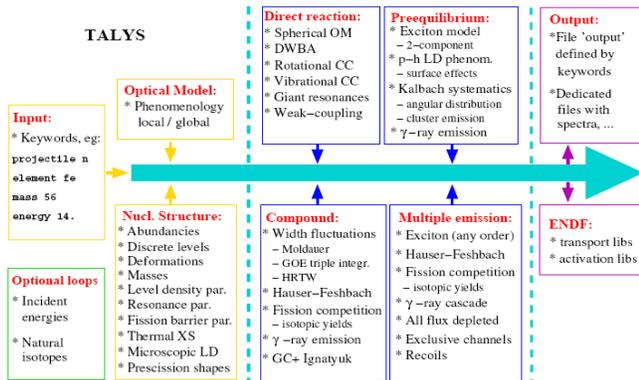


Fig. 2. Talys physic models modules

other extreme attitude that every nuclear reaction process which is expected to take place in reality should be present in a nuclear data library, having been experimentally measured or not. This imply a more robust reliance on nuclear modelling capacity for all open reaction channels, primary and secondary events. Where possible, and preferably, results based on model could still be over-ruled if strictly necessary by experimental information if those are of sufficient quality.

The TALYS/T6 system is in essence a technology suite of sequential and/or parallel processes that from basic atomic, mass and nuclear structure model, assemble and build the physical quantities that are necessary to evaluate nuclear data forms. The tip of the system infrastructure are the TALYS/T6 codes, briefly described above but upon a deeper inspection reveal no less than 58 codes executable, compiled and linked with their respective databases. Upon re-engineering and machine learning that number will inevitably and fortunately decrease.

### II.A.1. Thermal, resolved and unresolved ranges

The resolved and unresolved resonance range, named RRR and URR, respectively, are of major importance for the correct simulation of all systems that rely on thermal reactions at temperature. The goal there is to provide TALYS with a set of resonance parameters for all the target isotopes included in a TENDL neutron sub-library. Methodologies and processes are put in place to provide resonance parameters in all cases, when essential measurements exist allowing for a correct formalism to be implemented or not, on stable or radioactive targets. It should be clear that the following three cases can occurs and are handled appropriately.

- differential precise measurements/transmission data are available: resonance parameters in the ENDF-6 format (called MF-2 or file 2) are produced. Three for-

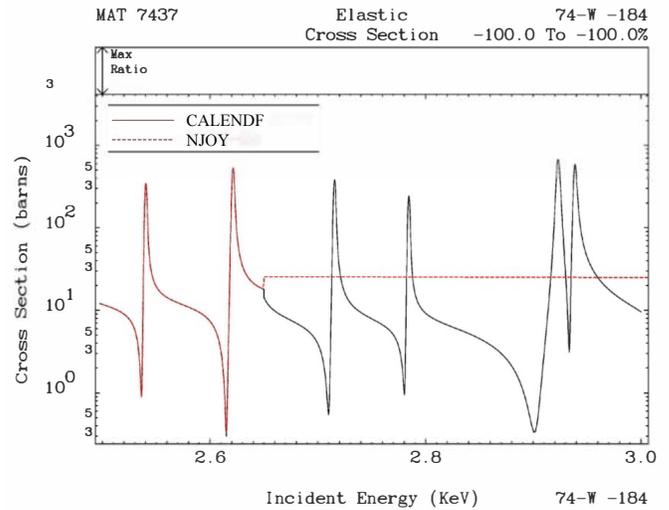


Fig. 3. CALENDF<sup>4</sup> statistical elastic resonances in the URR of  $^{184}\text{W}$

malism can be used: multi-level Breit Wigner, Reich-Moore, single-level Breit Wigner

- scattered, unprecise, incomplete measurements exists: resonance parameters are also produced, but with far less certainty
- no data: in this third case the High Fidelity Resonance approach or HFR<sup>5</sup> is applied, statistical resonance are outputted by the CALENDF<sup>6,7</sup> code, with 2813 targets this represent the majority.

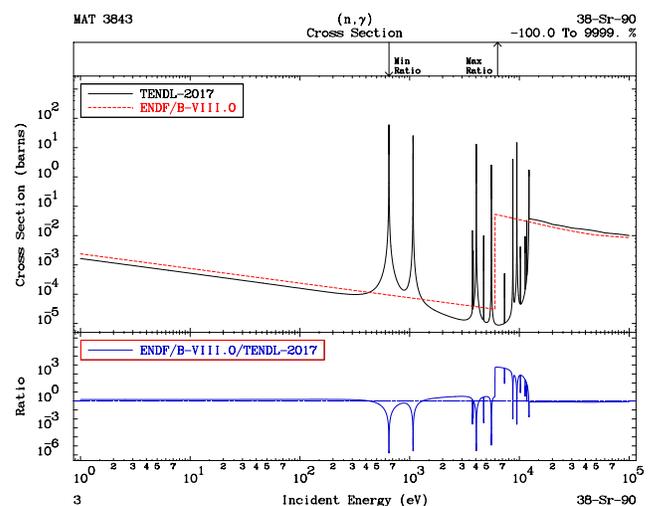


Fig. 4. Example of smooth and CALENDF statistical resonance cross sections for  $^{90}\text{Sr}(n,\gamma)$ : comparison between TENDL-2017 and ENDF/BVIII.0.

### II.A.2. Fast ranges

As mentioned in the introduction, above the resonance range, the nuclear reaction code TALYS is used to calculate all necessary quantities: cross sections, angular distributions, emitted spectra, double differential data, etc. The model code infrastructure has been used for many different applications, among which the production of the TENDL libraries.

The default calculations are based on a selection of reaction models and their parameters (e.g. the Koning-Delaroche optical model). Such parameters have been globally fitted to existing differential measurements as included in the EXFOR database. Once the values of such parameters are chosen to globally reproduce observables, they can also be used when no experimental information exist, with a dependence on the isotope characteristics. Apart from this global fitting, a specific isotopic approach is performed for isotopes which are technologically relevant. In such cases, local parameter values are used to more precisely reproduce experimental data.

Such dedicated evaluation process is time-demanding, but once it is done, the local parameter values are kept and stored in a database included in TALYS/T6 and recorded in the MF-1 of each evaluation. This way, every new releases of TENDL is started using these sets of already determined model parameters. Finally, there exists cases where the reaction models are not able to reproduce the observable, for instance because of model defects. In such cases, a procedure to normalize the TALYS simulation results to the observable is used. The approach is as follows: first obtain a fit with pure parameters leading to a nuclear data set as close as possible to the selected observable, then apply the necessary normalization directly to the observable. The advantage of this procedure is that the other, not experimentally observed or observable reaction channels are also derived from a consistent set of TALYS model simulations.

With such tools in hand, high-quality evaluations are obtained and conveniently reproduced in the fast energy range.

### II.B. Evaluated nuclear data structure

One major important, too often undermined in the past, aspects of nuclear data has been the format, structure in which such considered basic physic information would be stored and distributed. From the beginning the flawless physics needed to find its way into evaluation before been processed into applications forms, from the physic to engineering forms. Continental flavour established their ways, encouraged by the dogmatism, rigidity of the ENDF-6 format frame, targeted at two specific applications and the data forms they deemed necessary to better serve

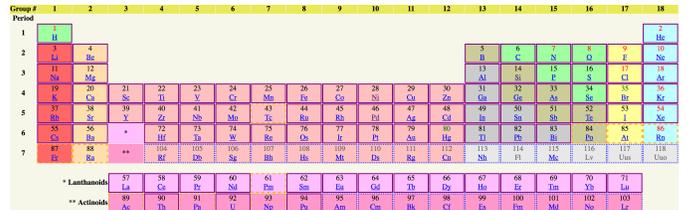
Sub-library	Targets	$E_{max}$
Neutron	2813	200
Proton	2808	200
Deuteron	2808	200
Triton	2808	200
He <sub>3</sub>	2808	200
Alpha	2808	200
Gamma	2808	200

**TABLE I.** TENDL-2017 neutron and charge particles library<sup>2</sup>

them.

In contrast TENDL structures, forms<sup>2</sup> are multiple but coherent. They serve, deliver for many different research fields ranging from astrophysics to medical or earth sciences. Those forms are:

- physic tables, X-Y format for cross section, emitted spectra and angular distribution
- $S_0$  ENDF-6 forms, single reaction channel: MF-3/MT-5\*MF-6 to 200 MeV
- $S_{30}$  ENDF-6 forms, multiple reaction channels: MF-3/MT-1 to 891\*MF-4/MF-5/MF-6 to 30 MeV, then as  $S_0$  afterwards
- Model based variance-covariance information, ENDF-6 forms MF-32, -33, -40



**Fig. 5.** TENDL-2017 neutron induced landscape

### II.C. Application forms

Considerable experience and know-how has been acquired on basic nuclear data since the dawn of the nuclear age, however some of this achievement has been done through fitting, profiling the underlying cross section with the essential and available at the time experimental information. The experimental set up were numerous, pioneering and founding, they shaped our actual knowledge and allowed the safe development of nuclear fission applications. Such methodology, fit for the purpose it was designed for came at a price: a proper, correct in term of physics, understanding of the compensation, correlation

at play throughout the complex simulation processes. Most often cross section adjustment is still considered an acceptable, inevitable step. Is that a safe approach for novel applications? when one may notice that 90% of the integral experiments used include bias of nature to disqualify them.

Tremendous progress, in term of simulation capability, granularity, accuracy and rightfulness has been achieved since then enabling more detailed and probing aspects of the underlying physic to be unearthed and revealed. Since mostly the turn of the century simulation probe has allowed to highlights certain sort-cut taken, deficiency, insufficiency. Fortunately, when no, little or contradictory experimental information exists models based on solid underlying physics interpretation are available. Physics model<sup>8</sup> allow to extend, supplement and enhanced the basic nuclear data so necessary to the modern applications. Physical models also allow to go where no experiment could go, usually with uncertainty.

With this understanding and the enhanced processing capabilities available through the latest generation of processing codes: NJOY-2016<sup>9,10</sup>, PREPRO-2018<sup>11</sup> and CALENDF-2010<sup>12</sup> it is now possible to provide multi-physics, multi-scale simulation with the nuclear data forms they so need to probe deeper, better into the experiments and advance safely in uncharted, novel territories. Continuous cross section with probability tables in the unresolved resonance range, adequately tabulated angular and emitted distributions spectra across all the incident energies, residuals and particles emissions channels; charge particles and residual matrices; isomeric state residuals and targets, non-elastic channels, isotopic and elemental correlation, long range variances, cross isotopes correlation are all enhanced data forms that may not change the overall pretty good criticality picture but most certainly better represent the physics at play and so our understanding in numerous other applications.

Many enriched results can now be extracted from innovative simulation processes that rely on those enhanced data forms and this well outside the paved paths in terms of applications, targets, incident particles, energy distributions, primary, secondary and time dependent responses.

- Advanced, alternative shielding materials
- Detailed reactions rates
- Non-criticality metrics, instrumentation
- Comprehensive emitted particles and recoils distributions
- Innovative material science metrics

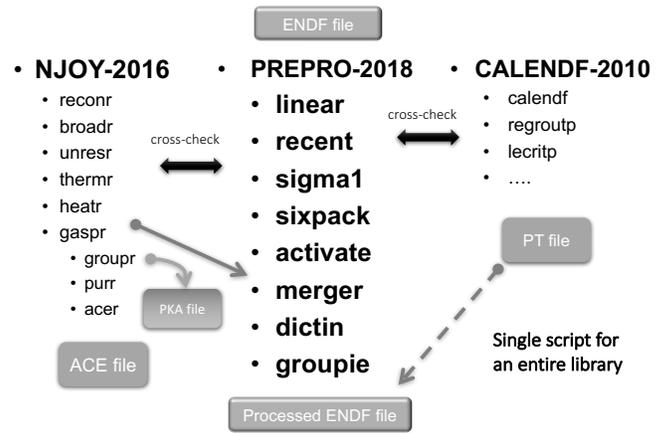


Fig. 6. Enhanced processing steps, three codes<sup>10-12</sup>

- Proper isomeric accountancy, down to the ms
- Primary (instantaneous) and secondary (decay) source terms
- Full time inventory, from milli-second up to millennia
- Decommissioning, storage monitoring
- Uncertainty quantification and propagation

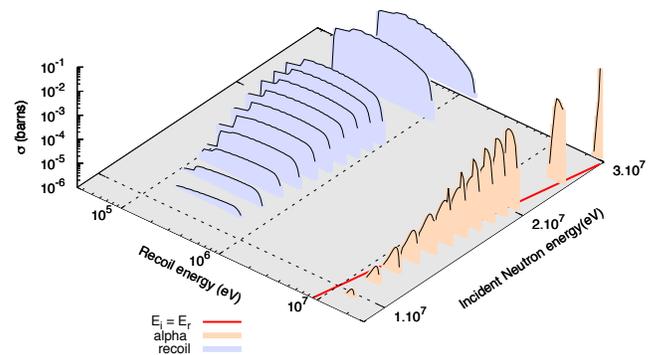
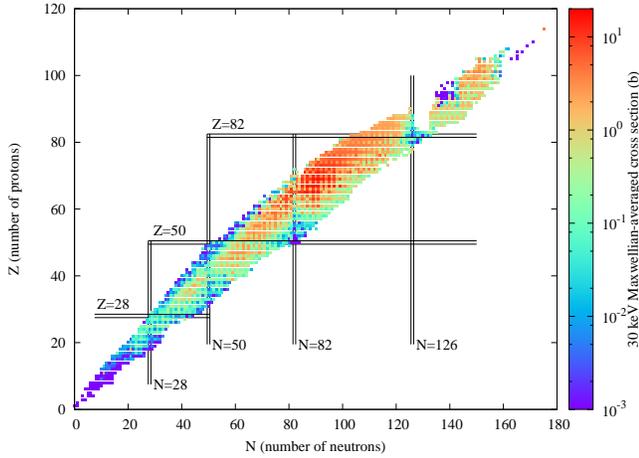


Fig. 7. Q positive (7.3 MeV) (n,  $\alpha$ ) <sup>184</sup>W, residual <sup>181</sup>Hf (blue), emitted <sup>4</sup>He (orange) energy spectra<sup>9</sup>, neutron incident energy in red, note the alpha energy superior to the neutron incident one, the spectra truncation above the 30 MeV upper energy

TENDL-2017<sup>2</sup> encompasses 2813 target nuclides, including some 543 isomeric states ( $T_{1/2} \geq 1s$ ), for seven incident particles alpha, gamma, deuteron, proton, helium, triton and neutron up to 200 MeV. Through its making, TENDL describes all open reaction channels, product yields, emitted spectra, short-lived daughter radionuclides

( $T_{1/2} \geq 0.1s$   $1/10_{th}$  of target half-life setting) and includes complete variance-covariance information derived from reference input parameters variation.



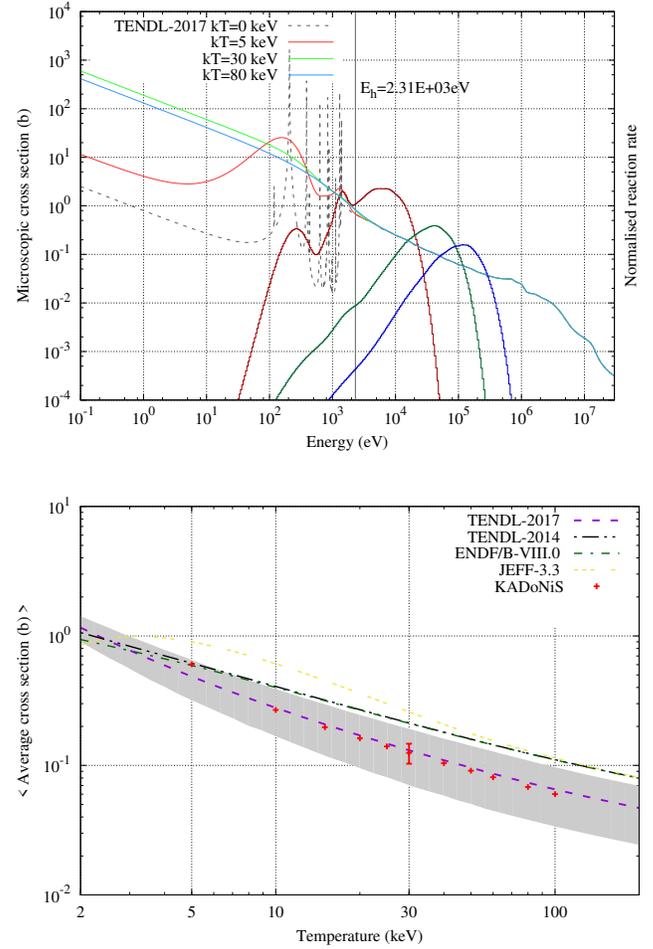
**Fig. 8.** 30 keV  $(n,\gamma)$  MACS for all nuclides in TENDL-2017. Magic numbers are identified by lines to help interpretation. MACS lower than 1 mb are given as the lower plot cutoff of 1 mb.

When fed into a modern simulation platform such as FISPACT-II<sup>13,14</sup>, as Bateman solver or MCNP<sup>15</sup>, SERPENT<sup>16</sup>, and OpenMC<sup>17</sup> as Boltzmann solvers, and applied to analysis and methodology in support of shielding, source terms and time inventory, those enhanced, complete data forms enable detailed and probing study of the nuclear landscapes like no other; leading more safely, securely and in details the way into uncharted, still un-probed territories, well beyond the legacy scenarios already commissioned. This is most potent when yet no experimental information pave the way.

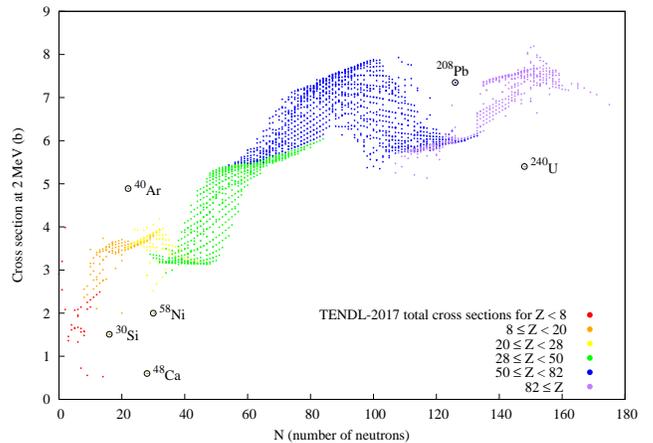
### III. CONCLUSIONS

Due to the methodology behind, enshrined in the TALYS/T6 system the TENDL libraries are annually updated and upgraded. This has resulted in a technologically generated nuclear data system that, with just 10 years of development, outperform the well-established, well-trodden legacy libraries for a large variety of applications. Those technological processes and mass data mining enable TALYS/T6 to be self-healing, constantly improving, responding quickly, with better physics and reproducibly to any new challenge it faces.

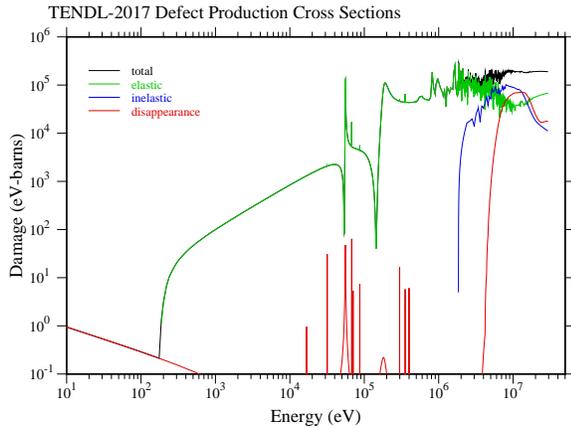
Shielding applications are now benefiting from a wider range of traditional and exotic isotopes, elements, materials, reliable and complete primary and secondary source terms, broad incident energy range and multiple entrance particles



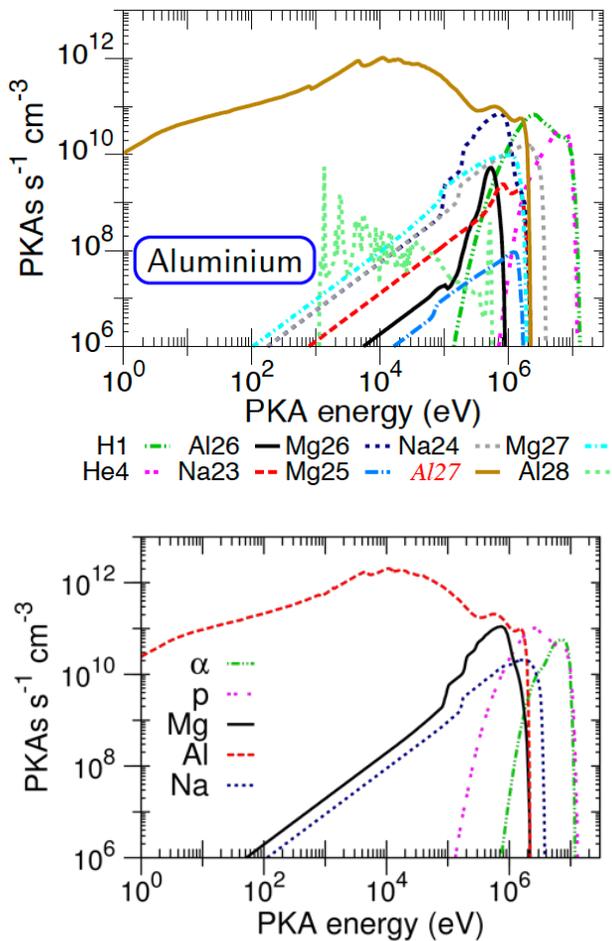
**Fig. 9.**  $^{205}\text{Pb}$  maxwellian-averaged capture cross sections for  $kT=1$  keV to 100 keV, KADoNiS, TENDL-2017,-2014, ENDF/B-VIII.0, JEFF-3.3, TENDL uncertainty in grey



**Fig. 10.** Total cross sections for all TENDL-2017 at 2 MeV, plotted against N and with Z broken down by magic number boundaries. Some potential outliers are highlighted.



**Fig. 11.** Example of radiation damage energy productions for  $^{28}\text{Si}$ , note the different components



**Fig. 12.** Isotopic and elemental residual Primary Knock on Atoms energy, n-induced on Aluminum, extended during processing at low energy for non-elastic events<sup>9,18,19</sup>

channel enabling them to truly probe the uncharted and efficiently optimise the existent.

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