The Database of Maxwellian Averaged Neutron Capture Cross Section (MACS) of the CERN Neutron Time-of-flight Facility (n_TOF) for Nuclear Astrophysics

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Abstract

We construct a database for all available isotopes' Maxwellian-Averaged Cross-Sections (MACS) measured at CERN n_TOF facility. In addition to the experimental data, the database contains theoretical values calculated by the `TALYS`*-2.0 program, as well as evaluated values from other libraries, for reference. Quantities such as Q-value, reaction rate, and stellar enhancement factor (SEF) are included for completeness. Our programming enables quick updates and modifications to data, with the entire process automated. It requires minimal input and provides a high degree of freedom to add comments or change the plotting style. The database contains complete information ready for theoretical simulation of nuclear-astrophysical processes, and MACS measurements at the CERN n_TOF facility are, to our knowledge, the newest and of high resolution.*

Keywords: nuclear astrophysics, nucleosynthesis, s-process, online database, neutron capture cross sections

1. INTRODUCTION

The neutron capture process has been hypothesized to be one of the fundamental processes of stellar nucleosynthesis Burbidge et al. (1957). The measurement of cross sections becomes important for the study of astrophysics, and KADONiS has attempted data collection Dillmann et al. (2014). Meanwhile, a significant amount of experimental work related to nucleosynthesis studies has been conducted at the CERN n_TOF facility. However, the key results from these activities have not yet been compiled for inclusion in major databases. To address this gap, we propose the establishment of a new database based on these measurements. In this letter, we outline the workflow for constructing the database and highlight some of its important features. While data storage is typically managed using an SQL system, we have opted for a different approach utilizing Python programming, which is simpler and easier to maintain. Section 2 provides a brief overview of the theoretical aspects of the neutron capture process and defines key quantities. Detailed information about the workflow and features of the database can be found in Section 3.

2. MAXWELLIAN-AVERAGED CROSS SECTIONS

The origin of the chemical elements present in the universe has been a subject of extended investigations for the past sixty years Burbidge et al. (1957). All the trans-iron elements are believed to have been synthesized through nuclear reaction processes involving neutron capture and beta decays, during various phases of stellar evolution.

2.1. Neutron Capture Process

Accurate energy-averaged neutron capture cross sections are needed to establish the quantitative details of these processes. In particular, a process called the s-process, responsible for the formation of about half of the heavy elements present in the universe, requires accurate determination of neutron capture cross sections Burbidge et al. (1957). Neutrons produced in stellar interiors quickly reach thermal equilibrium, whose velocities are described by a Maxwell-Boltzmann distribution. This report and the database focus on the neutron capture process $A + n \to B + \gamma$, commonly represented as $A(n, \gamma)B$. The nuclear reaction Q-value is defined to be the mass difference of the nuclei at the entrance channel and that at the exit channel, which we also include in our database.

2.2. Cross Section

In addition to the reaction Q-value, the cross-section provides dynamic information of 2-2 collision. Its definition is intuitively

$$\sigma = \frac{1}{T}\frac{\text{number of scattered particles}}{\text{particle flow}} \tag{1}$$

We also define the reaction rate per nucleus and neutron pair, where v is the relative velocity

$$\langle\sigma v\rangle = \int_0^\infty \int_0^\infty dv_A dv_n\, \phi(v_A)\phi(v_n)\sigma(v)v \tag{2}$$

If an incoming neutron possesses relative orbital angular momentum, which can be directly associated with the impact parameter $\ell = p_{\rm re}b$ in the laboratory frame, it will need to overcome a centrifugal barrier due to the conservation of angular momentum. At thermal neutron energy $Q \gg E_n$, the nuclear reaction is dominated by the neutrons with $\ell = 0$. Then, the cross section at this approximation is proportional to the inverse of the relative velocity

$$\sigma(E_n) \propto \frac{1}{v}. \tag{3}$$

Therefore, the reaction rate is approximately a constant

$$\langle \sigma v \rangle = \text{constant} = \langle \sigma \rangle v_T. \tag{4}$$

We define the Maxwellian-averaged cross-section (MACS) $\langle \sigma \rangle$ as the ratio of this with the most probable thermal velocity v_T. The MACS can then be calculated with the relation

$$\langle \sigma \rangle = \frac{\langle \sigma \cdot v \rangle}{v_T} = \frac{2}{\sqrt{\pi}} \frac{1}{(kT)^2} \int \sigma(E) E \exp(-E/kT) dE \tag{5}$$

where the velocity of the relative motion between the neutron and the target nucleus has been transformed into its kinetic energy E, and kT is the thermal energy (or temperature) at which the neutron capture reaction is taking place. The neutron capture cross section $\sigma(E)$, as a function of the incident neutron kinetic energy, needs to be known from either experiments or nuclear reaction model calculations across a wide range of neutron energies.

2.3. Stellar Enhancement Factor

Current available measurements of MACS are conducted in a laboratory environment, where the neutron beams can cover a wide energy range while the target nuclei are in their ground state. However, in the stellar environment, the nuclei can also be thermally excited. Therefore, in the determination of appropriate nuclear reaction rates, we should incorporate the population probabilities for nuclei at various excited states, which are labeled by their excitation energy E and angular momentum J, at the specified thermal energy kT, c.f.(Mengoni (2020)).

$$\sigma_{\text{STAR}}(n, \gamma) = \sum_{i=0}^{N} p_i \sigma_i(n, \gamma). \tag{6}$$

where

$$p_i \equiv \frac{(2J_i + 1) \exp(-E_i/kT)}{\sum_{i=0}^{N} (2J_i + 1) \exp(-E_i/kT)} \tag{7}$$

are the probabilities for populating any nuclear state $\{E, J\}$, $i = 0, \cdots, N$. In this notation, the MACS measured in the laboratory is $\sigma_{\text{LAB}}(n, \gamma) = \sigma_0(n, \gamma)$.

We can define the ratio of MACSs between the stellar and the laboratory as *stellar enhancement factor*,

$$\text{SEF} \equiv \frac{\sigma_{\text{STAR}}(n, \gamma)}{\sigma_{\text{LAB}}(n, \gamma)}. \tag{8}$$

The SEF included in the database is calculated directly from the output of TALYS calculations, by the ratio of equation 8.

3. THE n_TOF@CERN ASTROPHYSICAL MACS DATABASE

3.1. The KADoNiS Project

The Karlsruhe Astrophysical Database of Nucleosynthesis in Stars (KADoNiS) project is a leading initiative for compiling astrophysical nuclear data. Established in 2005, KADoNiS is an online database that provides recommended cross-sections essential for studying nucleosynthesis in stars. The primary *s*-process database includes a comprehensive collection of Maxwellian-average cross sections (MACS) for neutron capture reactions. Its core content consists of recommended MACS values at a thermal energy of $kT = 30$ keV for over 360 isotopes, ranging from hydrogen (H1) to bismuth (Bi210). For isotopes lacking experimental data, the database provides semi-empirical values derived from theoretical calculations that are adjusted to align with the systematics of neighboring nuclei. It also lists available experimental data and allows users to compare it with predictions from major evaluated nuclear data libraries. The KADoNiS project aims to provide researchers with access to experimental data relevant to astrophysical energy regions. This resource is critical for nucleosynthesis modeling and for benchmarking theoretical predictions.

3.2. Architecture of n_TOF Astrophysical Database

Inspired by the KADoNiS project, we have created an online database with the most recent measured MACS at the n_TOF facility. Visit our website for more information. Most of the technical details, programming, and instructions can be found in this GitHub repository.

In this subsection, we introduce the architecture of the n_TOF astrophysical database, its current features, and some future functions we are interested in developing. For starters, the workflow consists of three main parts: evaluating and merging MACS data, plotting the comparison of MACS results, and deploying the static webpages. The workflow chart is shown in Fig. 1. The user must provide two input files at different stages when attempting to append new data/or to modify old data to the database. Let's first focus on evaluation and merging data. The input file must incorporate the most recent MACS data measured at n_TOF. Furthermore, if feasible, it is recommended to include references and details regarding the n_TOF collaboration as comments. An example of the nucleus Au197 is illustrated in Fig. 2.

Annotations or footnotes related to this isotope can be included, and they will appear in a box on the datasheet, which we will review the layout of later. Note that they should be in the `HTML` format.

The specific range of temperatures is further extracted to evaluate the theoretical MACS with `TAYLS-2.0` program (Koning et al. (2023)) with default setup. Quantities such as SEF and Q-value are either evaluated with this program or extracted from its built-in dataset[1]. On the other hand, the reaction rate is

[1]We use Eq. 6 to evaluate the MACS in the stellar environment and then compute the SEF.

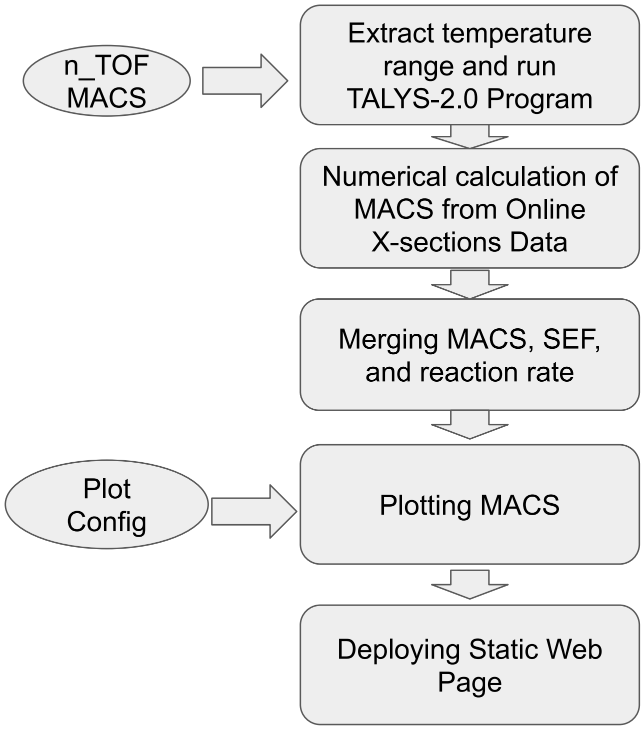


Figure 1: Data processing pipeline for the n_TOF astrophysical database, showing the integration of theoretical calculations (TALYS-2.0), data merging, and web deployment for MACS and reaction rates.

evaluated with the MACS measured at n_TOF,

$$\langle \sigma v \rangle = \langle \sigma \rangle v_T \tag{9}$$

Additionally, there are experimentally evaluated data of cross sections measured at different laboratories, and the MACSs computed from these measured cross sections are classified as *evaluated value* in our database. Laboratories of measured cross sections at default are `ENDF/B-8.1`, `JEFF-3.3`, and `JENDL-5`, but one can include whatever laboratories of measured cross sections and evaluated MACS with slight modifications in the `Python` code we provided. There can also be some existing direct experimental MACSs (like `KADoNiS` (Dillmann et al. (2014)) we mentioned), together with n_TOF MACSs, classified as *experimental value*. Then, we combine the experimental values, the theoretical value, the evaluated value of MACS, SEF, and the reaction rate at different temperatures into one `csv` file, which is used to build the table in the datasheet on the website, as shown in Fir. 3. Next, the input file for the plotting functions contains the configuration of plotting styles for different MACS values of each nucleus, where the user can customize these settings. This is important because experimental MACSs, except that of n_TOF, may be available for some nuclei while not for others. Moreover, we provide an option to plot the uncertainty, which is often turned on for experimental values. This input file should be in the `JSON` format, as shown in Fig. 4. Additionally, we provide the plot of the ratio to the n_TOF MACS, following the same plotting configuration as the MACS comparison plot, as shown in Fig. 5a and 5b.

Last but not least, we implement a `Python` code with `FLASK` and `FROZEN-FLASK` package to deploy our website. The website also contains three main parts: the home page, the item list (or search result list), and the datasheet page. The home page provides an overview of the database's features, accompanied by a search functionality and a complete catalog of all available items, enabling users to access the full dataset. A downloadable text file of all n_TOF MACS values is available on the home page in ASCII format, as shown in Fig. 6. Currently, individual n_TOF MACS values can only be accessed per nuclide from their respective data sheets, as shown in Fig. 7. The datasheet page is divided into several sections. First, it provides downloadable n_TOF data in `ASCII` format, along with a valid reference link to the publications in the comment box. There is the comment box left with basic properties, such as the Q value, and the MACS30 measured at n_TOF, as well as special comments on the MACS. Second, a table is provided that includes MACS from various sources, as well as SEF and reaction rates at different temperatures between $kT = 5$ and 100 keV. Finally, we provide the comparison plot of MACS from different sources and useful links to other valid resources.

3.3. A User-friendly Interface and Fast Implementation System

As we previously mentioned, updating the new MACS data or modifying the old MACS data in this setup is fast and simple. Two input files are required: one providing the experimental Maxwellian-Averaged Cross Sections (MACS) data at n_TOF, which may also contain experimental MACS from sources such as KaDONis or other relevant databases; and a second file containing the plotting configurations. The first input file should also include a brief description of the relevant publication, along with the reference link to the n_TOF collaboration. Users are encouraged to include any special comments related to the n_TOF MACS. There is no limit on the reference links, which is a useful feature for future development on version control and updating old data sheets. The plotting configuration file enables users to customize the presentation and visualization parameters of the MACS data. Then, after preparing input files for each nucleus, one can run the provided `run.sh` script, which will go through the workflow for a single isotope. In addition, we also provide a script `run_batch.sh` for a batch of data, and the example usage is shown in Fig. 8.

```
./run.sh {element} {mass} {format-hint}
./run_batch.sh jobs.txt
```

Figure 8: Command-line interface for the processing scripts. The `run.sh` script processes a single nucleus, while `run_batch.sh` handles a list of jobs from a file, enabling both individual and high-throughput calculation of MACS and reaction rates.

Where `format-hint` would indicate the significant digit of the MACS value measured at n_TOF, and the text file `jobs.txt` contains multiple lines of `{element} {mass} {format-hint}`. The corresponding datasheets and plots would be created in the `build` folder, and the files can be deployed immediately to the cloud.

```
# Main Publication of the n_TOF Collaboration : <br>Au197(n,g) cross section in the unresolved resonance region<br>C. Lederer, N.
↪  Colonna, C. Domingo-Pardo, F. Gunsing, F. Käppeler, C. Massimi, A. Mengoni, A. Wallner, U. Abbondanno, G. Aerts et al. (The n_TOF
↪  Collaboration)<br>Physical Review C 83, 034608 (2011)
# Comment : <br>n_TOF full energy range
# REF https://doi.org/10.1103/PhysRevC.83.034608
kT (keV),n_TOF (mb)
6.0,1729 ± 61
7.0,1550 ± 54
8.0,1412 ± 49
...
```

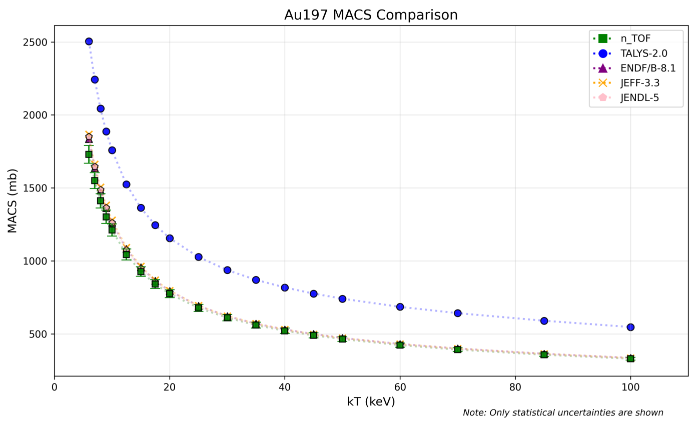
Figure 2: Example of the structured input data (CSV format) used by the database pipeline, showing MACS values and uncertainties for the ^{197}Au(n, γ) reaction at different thermal energies (Lederer et al. (2011)).

```
# Au197
# Q value : 6.512 [MeV]
# MACS (n_TOF) @ 30 keV : 611 ± 22 [mb]
# Main Publication of the n_TOF Collaboration : <br>Au197(n,g) cross section in the unresolved resonance region<br>C. Lederer, N.
↪  Colonna, C. Domingo-Pardo, F. Gunsing, F. Käppeler, C. Massimi, A. Mengoni, A. Wallner, U. Abbondanno, G. Aerts et al. (The n_TOF
↪  Collaboration)<br>Physical Review C 83, 034608 (2011)
# Comment : <br>n_TOF full energy range
# REF : https://doi.org/10.1103/PhysRevC.83.034608
kT (keV),n_TOF (mb),TALYS-2.0 (mb),ENDF/B-8.1 (mb),JEFF-3.3 (mb),JENDL-5 (mb),Reaction_rate (cm³/mol/s),SEF
6,1729 ± 61,2504,1836,1867,1852,1.12E+08,1.00
7,1550 ± 54,2243,1636,1662,1646,1.08E+08,1.00
8,1412 ± 49,2044,1483,1505,1488,1.05E+08,1.00
...
```

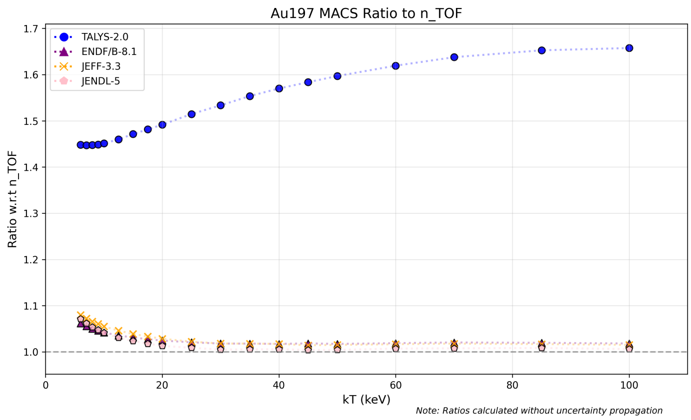
Figure 3: Consolidated data file for the ^{197}Au(n, γ) reaction, merging experimental, theoretical, and evaluated MACS values with calculated reaction rates and SEF. This format serves as the direct input for populating the interactive data tables on the website.

```
[
    {
        "column": "n_TOF (mb)",
        "label": "n_TOF",
        "color": "green",
        "marker": "s",
        "with_unc": true,
        "line_style": ":",
        "line_width": 2,
        "line_alpha": 0.3,
        "marker_size": 50
    },
    {
        "column": "TALYS-2.0 (mb)",
        "label": "TALYS-2.0",
        "color": "blue",
        "marker": "o",
        "with_unc": false,
        "line_style": ":",
        "line_width": 2,
        "line_alpha": 0.3,
        "marker_size": 50
    },
    ...
]
```

Figure 4: Visualization configuration file in JSON format. The objects within the array specify the plotting properties—such as color, marker, and line style—for the corresponding data columns in the combined CSV file, enabling consistent and customizable graphical representation.



(a) Comparison of Maxwellian-averaged cross-sections (MACS) for the ^{197}Au(n, γ) reaction. The n_TOF experimental data are shown with statistical uncertainties and compared to TALYS-2.0 predictions and major evaluation libraries.



(b) Ratio of theoretical and evaluated MACS values to the n_TOF data for ^{197}Au(n, γ). Ratios are calculated using central values without uncertainty propagation.

4. CONCLUSIONS

The Maxwellian-Averaged Cross-section (MACS) is crucial for understanding the formation of heavy elements, those that are heavier than iron, during stellar evolution. The CERN n_TOF database contains such quantities, as well as valid, citable references, and is useful for astrophysical simulations and phenomenology. In the future, we plan to develop a more user-friendly graphical interface and version control that in-

```
# kT [keV]          au197_macs [mb]          unc [mb]
6.0        1729          61
...
# kT [keV]          ce140_macs [mb]          unc [mb]
5.0        34.37          0.24
...
# kT [keV]          ge76_macs [mb]          unc [mb]
5.0        65.0          3.3
...
```

Figure 6: Excerpt of the master ASCII file providing all n_TOF MACS values. The data for each isotope is grouped, listing temperatures, cross-section, and uncertainty, serving as the primary data export for users.

```
# Au197 Maxwellian-Averaged Cross Sections (MACS)
# REF https://doi.org/10.1103/PhysRevC.83.034608
# Cross sections and uncertainties in millibarns (mb)
# kT [keV]          n_TOF [mb]          ± uncertainty [mb]
6.0        1729          61
7.0        1550          54
8.0        1412          49
...
```

Figure 7: Per-nuclide data file format for the ^{197}Au(n, γ) reaction. This structured `ASCII` output provides the n_TOF MACS values and their uncertainties at specific temperatures, available for individual download from each isotope's data sheet.

cludes more detailed data. In conclusion, we have developed a database that compiles the Maxwell-Averaged Cross Sections (MACS) measured at the CERN n_TOF facility together with reference data evaluated from various nuclear libraries. In addition, we provide plots of the MACS values and their ratios with respect to the n_TOF measurements to illustrate the differences. The data have been standardized into an `ASCII` format to enable immediate use.

ACKNOWLEDGEMENTS

The author gratefully acknowledges the support provided by the CERN Non-Member State Summer Student Programme. Special thanks to Professor Alberto Mengoni for his invaluable supervision, technical support, and insightful discussions throughout the project, as well as for his constructive feedback on the manuscript.

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