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The new KADoNiS v1.0 and its influence on the weak s-process nucleosynthesis

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Five years after the release of KADoNiS v0.3 (www.kadonis.org), a major update on the *s*-process database has been completed and is presently available for testing at HTTP://EXP-ASTRO.PHYSIK.UNI-FRANKFURT.DE/KADONIS1.0/. All available datasets between ^{1}H and ^{210}Bi and their energy dependence for kT= 5 - 100 keV have been reviewed, updated, and evaluated. The main difference to previous releases of KADoNiS is the intensive work that has been put in the inclusion of new experimental energy-dependent cross sections which should make the extrapolations to higher and lower energies more reliable. Also a revision of the ^{197}Au(n,γ) cross section has been applied which is widely used as reference cross section for time-of-flight and activation measurements. Several recent measurements in the astrophysical energy range have led to a new recommended value used throughout KADoNiS v1.0 which is $3-5.4\%$ higher than the previously adopted value.
Datasets for the up to now missing light stable isotopes ^{6}Li, ^{10,11}B, and ^{17}O were added and recommendations based on experimental data given. The total number of datasets in the KADoNiS database increased from 370 to more than 440 which is mainly due to the inclusion of radioactive isotopes 1-2 mass units away from stability. Although no measurements are available for these cases, they play an important role in modern *s*-process calculations with higher neutron densities. To be able to use a consistent database for *s*-process simulations it was decided to include these isotopes in the new update and calculate semi-empirical recommended cross sections.
In this update also indirect measurements, namely (γ,n) measurements complemented by Hauser-Feshbach predictions with constrained input, have been included which yielded new (n,γ) recommended values for e.g. the branchings at ^{85}Kr, ^{185}W, and ^{186}Re. For other branching isotopes, e.g. ^{63}Ni, first direct experimental time-of-flight data yielded a factor of 2 higher cross section compared to the previously used theoretical prediction.

The influences of the changes of the new (n,γ) cross sections on the weak s-process have been investigated. Whereas the differences after core He burning are within 20%, the impact of the new set of MACS on the *s*-process abundance distribution is much larger at the end of the shell C burning which leads to a "weaker" *s*-process efficiency.

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1. The KADoNiS *s*-process database

An important ingredient for reliable *s*-process simulations are accurate cross sections for the participating nuclei [1]. For example, in massive stars the uncertainties of single neutron-capture cross sections in the weak *s*-process (60<A<90) can produce a long-range propagation effect which affects the whole reaction flow up to the next shell closure at N=50 since no local equilibrium exists in the weak component (the product abundance times cross section for neighboring isotopes in the reaction path is no longer approximately constant). This was first demonstrated for ^{62}Ni(n,γ) [2] where until five years ago experimental values at stellar temperatures (kT=30 keV) ranged between 12 and 37 mb. The higher cross section produces a 45% higher yield of all isotopes between A=65 and 90 in stellar models compared to the previously recommended value of 12 mb. A careful analysis including new measurements has led to a new recommended value of 22.2$\pm$1.3 mb at kT=30 keV in KADoNiS v1.0 [3].

Important nuclei in the *s* process, where accurate cross sections are indispensable, are isotopes at the neutron shell closures and the so-called "*s*-only isotopes". The latter are mostly of pure *s*-process origin and thus represent a unique probe of the *s*-process abundance distribution. The desired uncertainty at stellar temperatures is <5% which is up to now only achieved for some isotopes between A=110-176. The isotopes at the shell closures are directly responsible for the *s*-process abundance peaks in the solar distribution because their small capture cross sections are hindering the reaction flux towards higher masses. The average uncertainty at kT=30 keV for all 19 stable isotopes at N=28, 50, 82, and 126 is presently $\pm$8.3%.

Robust *s*-process nucleosynthesis calculations for massive stars require an accurate knowledge of the neutron capture cross section of light neutron poisons (e.g. ^{12}C, ^{16}O, ^{20}Ne), since their impact on the neutron economy of the *s*-process depends on both, their abundance and their neutron capture rates. The propagation effect due to light neutron poisons was first discussed by [4] for ^{22}Ne.

The pioneering compilation for stellar neutron capture cross sections was published in 1971 by Allen and co-workers [5]. This paper reviewed the role of neutron capture reactions in the nucleosynthesis of heavy elements and presented a table of recommended (experimental or semi-empirical) Maxwellian averaged cross sections at kT= 30 keV (MACS30) for nuclei between carbon and plutonium. The idea of an experimental and theoretical stellar neutron cross section database was picked up by Bao and Käppeler [6] in 1987 for *s*-process studies. This compilation included cross sections for (n,γ) reactions between ^{12}C and ^{209}Bi, some (n,p) and (n,α) reactions for isotopes between ^{33}S and ^{59}Ni, and also (n,γ) and (n,f) reactions for long-lived actinides. A follow-up compilation was published in 1992 [7], and in 2000 the compilation [8] was extended to Big Bang nucleosynthesis. It included a collection of recommended MACS30 values for 364 isotopes and isomers between ^{1}H and ^{209}Bi, and semi-empirical recommended values for nuclides without experimental cross section information. These estimated values are normalized cross sections derived with the Hauser-Feshbach code NON-SMOKER [9], which account for known systematic deficiencies in the nuclear physics input. Additionally, the database provided stellar enhancement factors and energy-dependent MACS for thermal energies between kT= 5 keV and 100 keV.

The first version of the "Karlsruhe Astrophysical Database of Nucleosynthesis in Stars" (KADoNiS) was released in 2005 [10]. This online database was an updated sequel to the previous compilations. KADoNiS has been updated four times until now [11], with the present KADoNiS v1.0 being the most extensive update so far. The previously missing datasets for stable ^{6}Li, ^{10,11}B, and ^{17}O were included, and recommendations are given based on experimental data. The values from most recent evaluated libraries ENDF/B-VII.1 [12] and JENDL-4.0 [13] were included, and were used in many cases instead of older time-of-flight measurements. The total number of datasets in the new KADoNiS database increased by 20% to more than 440 which is mainly due to the inclusion of radioactive isotopes 1-2 mass units away from stability. Although no measurements are available for these cases, they play an important role in stellar *s*-process conditions associated to neutron densities of $>10^{10}$ cm^{-3}, or for neutron-capture process conditions intermediate between the *s* process and the *r* process (e.g., in the "intermediate (*i*) process" [14, 15]).

Only reactions on nuclei in their ground states (g.s.) are measured in laboratory experiments (with exception of quasi-stable ^{180}Ta^{m}). In the stellar environment, however, also reactions on thermally excited states of the nuclei contribute to the reaction rate. In the past, experimental g.s. rates have been converted to stellar ones using a stellar enhancement factor (SEF), given by the theoretically predicted ratio between stellar rate and g.s. rate. This approach has been found to be inadequate [16] and has been replaced by the procedure given in [17], which also allows to properly define uncertainties in the stellar rates from a combination of theoretical and experimental uncertainties. In the KADoNiS datasheet we show now both, the SEF and the new ground-state contribution labelled as "*X* factor".

All available datasets between ^{1}H and ^{210}Bi and their energy dependence for kT= 5 - 100 keV have been reviewed, updated, and evaluated. The main difference to previous releases of KADoNiS is the intensive work that has been put in the inclusion of new experimental energy-dependent cross sections which should make the extrapolations to higher and lower energies more reliable. However, this leads also to some remarkable differences compared to previous recommendations, some of which will be mentioned in this report.

2. The new recommended ^{197}Au cross section

Gold is commonly used as reference for neutron capture cross section measurements. However, it is considered as a standard only for thermal energy (25.3 meV) and in the energy range between 200 keV and 2.8 MeV [18]. For this reason the reference cross section used throughout previous versions of KADoNiS was based on an activation measurement of the Karlsruhe group [19] yielding a MACS of 582$\pm$9 mb at kT= 30 keV. The extrapolation to higher and lower energies was performed by using the energy dependence measured at the ORELA facility at Oak Ridge [20].

However, recent time-of-flight measurements at n_TOF [21, 22] and GELINA [23] revealed a 5% higher MACS at kT= 30 keV, in perfect agreement with the ENDF/B-VII.1 evaluation [12]. Including these measurements we have re-evaluated the ^{197}Au(n,γ) cross sections used in the KADoNiS database. The new recommended cross section for the astrophysical energy region was derived between *k*T= 5 and 50 keV by the weighted average of the GELINA measurement and the n_TOF measurement. The uncertainty in this energy range was taken from [23]. For the energies between kT= 60-100 keV we used the average of the recent libraries (JEFF-3.2, JENDL-4.0, ENDF/B-VII.1) and the uncertainty from the standard deviation given in JEFF-3.2 and ENDF/B-VII.1.

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The resulting new recommended dataset in KADoNiS v1.0 is given in Table 1. A comparison between the previous and the new recommended MACS between kT= 5 and 100 keV shows differences between 2.9 and 5.4%. The new cross section recommendation is also supported by a new activation measurement by the group in Sevilla [24] which reported a MACS30 of 619±30 mb.

kT (keV)	MACS (mb) KADoNiS v1.0	MACS (mb) KADoNiS v0.3	Ratio v1.0/v0.3
5	2109 (20)	2050	1.029
8	1487 (13)	-	-
10	1257 (10)	1208	1.041
15	943 (10)	904	1.044
20	782 (9)	746	1.049
25	683 (8)	648	1.055
30	613 (7)	582 (9)	1.053
40	523 (6)	496	1.054
50	463 (5)	442	1.048
60	425 (5)	406	1.048
80	370 (4)	356	1.039
100	332 (4)	321	1.033

Table 1: New recommended MACS of ^{197}Au(n,γ). The values given in brackets are the respective uncertainties (in mb).

3. Examples for major changes

Four examples for the impact of the new update on weak s-process nucleosynthesis are shown in Fig. 1. ^{63}Ni ($t_{1/2}$= 100 y) and ^{85}Kr ($t_{1/2}$= 10.76 y) are branching point nuclei in the weak s-process. The magnitudes of their neutron capture cross sections determine how much of the reaction flow is bypassing the s-process isotopes ^{63}Cu and ^{86}Sr. ^{63}Ni(n,γ) has been recently measured for the first time experimentally at n_TOF [25]. The new recommended cross section is more than a factor of 2 higher over the whole astrophysical energy range than the previously recommended semi-empirical value. For ^{85}Kr no direct measurement exists but the new recommended value was inferred from a recent photoactivation measurement of ^{86}Kr [26]. The new cross section is about 35% higher than the previous semi-empirical value.

For the weak s-process, ^{22}Ne$(\alpha,n)^{25}$Mg is the main neutron source during both burning phases, in convective core He burning at kT= 26-30 keV and later in shell C burning at about kT= 90 keV [27]. ^{25}Mg is the direct product of this source and is one of the major neutron poisons in massive stars. The new ^{25}Mg(n,γ) cross section is more than 40% lower than before, thus reducing the poisoning effect of ^{25}Mg.

At the end of convective core He burning as well as in the following evolutionary stage of C burning, ^{16}O is the most abundant isotope. Therefore, and despite its low neutron capture cross section, ^{16}O captures most of the neutrons made by the ^{22}Ne(α,n) neutron source. On the other hand, in He burning conditions ^{16}O(n,γ)^{17}O is followed by the ^{17}O$(\alpha,n)^{20}$Ne, recycling most of

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the neutrons captured by ^{16}O. The competition of the (α,n) channel with the ^{17}O(α,γ) is regulating the poisoning efficiency of the ^{16}O(n,γ) reaction in He-burning conditions [28]. The situation is different in C-burning conditions, where also proton captures are contributing to destroy ^{17}O, reducing the recycling efficiency of ^{17}O(α,n).

Therefore, in weak *s*-process conditions ^{16}O becomes an important neutron poison in the convective C-burning shell. In the new Kadonis release we include a re-evaluated ^{16}O(n,γ) cross section, which is ca. 10% lower at core He-burning temperatures, and 11% higher at C-burning temperatures [3, 29].

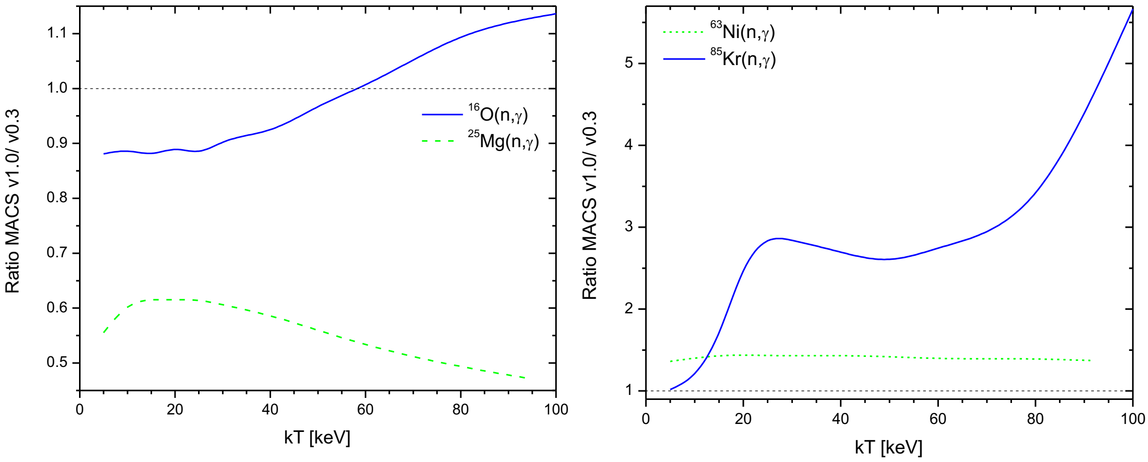

Figure 1: Ratios of new and previously recommended MACS between kT= 5-100 keV for ^{16}O and ^{25}Mg (left), and for ^{63}Ni and ^{85}Kr (right).

4. Weak *s*-process simulations

To investigate the effect of the new cross sections in KADoNiS v1.0 on *s*-process nucleosynthesis we have carried out a weak *s*-process study on representative trajectories selected from a 25 $M_\odot$ star. The nucleosynthesis calculations are done using the post-processing PPN code via the NuGrid Ubuntu Access virtual machine [30]. The resulting final abundances are shown in Fig. 2 as ratio of production factors using the previous cross sections based on KADoNiS v0.3 [11] and the new updated cross sections up to Z=50 (Sn) [3].

The majority of changes for core He burning are in the range of ±20%, with exception of the abundances of ^{58}Ni, ^{70}Zn, and ^{77}Se. These changes can be directly attributed to the changes in the new (n,γ) cross sections which are either higher (more destruction of ^{77}Se) or lower (less destruction of ^{58}Ni and ^{70}Zn).

The differences in shell C burning at higher temperatures are more pronounced, up to a factor of 2 for some isotopes like ^{76}Ge, ^{96}Zr, ^{58}Ni, ^{63}Cu, and ^{64}Cu. In particular, the production of isotopes up to Cu is comparable or higher, while most of nuclei between A=65 and 85 are less produced by about 60%. This "weaker" *s*-process in the mass region between Ge and Rb is mainly due to the new MACS for Ni and Cu isotopes, allowing to accumulate Cu and reducing the *s*-process flux toward heavier species. A stronger production of Cu compared to heavier *s*-process isotopes due to the new MACS was already indicated by [27]. The present calculations with the newest MACS (e.g., for ^{62}Ni and ^{63}Ni [25]) confirm this trend. Note that an overproduction of proton-rich isotopes and an underproduction of the respective neutron-rich isotopes is visible in many isotopic chains. This is due to the fact that the proton-rich isotopes are less destroyed by the *s*-process flux.

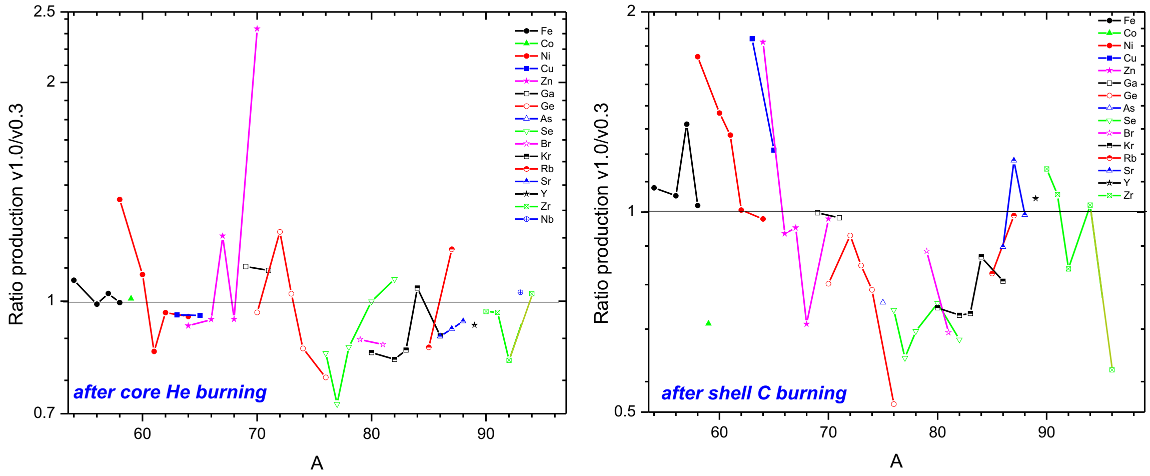

Figure 2: Abundance ratios from weak *s*-process simulations. Left: after core He burning. Right: after shell C burning. We show here stable and unstable isotopes with relative mass fractions of $X > 10^{-10}$.

5. Summary

The KADoNiS *s*-process database has undergone a major update in the last years and has been extended to more neutron-rich isotopes. The inclusion of experimental energy-dependencies will make the extrapolations to higher and lower energies more reliable for astrophysical simulations. A remeasurement of the ^{197}Au(n,γ) cross section at stellar energies revealed a discrepancy of up to 5.5% compared to the previously recommended values for $kT = 5-100$ keV. These new results led to a renormalization of several recommended cross sections of isotopes in the KADoNiS database. Only 8 stable isotope are left without any measurement at stellar energies: ^{17}O, ^{36,38}Ar, ^{40}K, ^{98,99}Ru, ^{138}La, and ^{158}Dy, while the overall number of datasets in KADoNiS without experimental information has increased from 90 to >150 isotopes due to the inclusion of many radioactive isotopes 1-2 mass units away from stability. The total number of datasets between ^{1}H and ^{210}Bi is now 443.

With the new set of recommended MACS up to Z=50 we have carried out weak *s*-process simulations. Whereas the differences between the previous and the new cross section database are not very strong during core He-burning (±20%), the higher temperatures during the following shell C-burning lead to differences up to a factor of 2. Further investigations are underway.

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