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UPDATING THE NUCLEAR REACTION RATE LIBRARY (REACLIB) I. EXPERIMENTAL REACTION RATES OF THE PROTON–PROTON CHAIN

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REACLIB is one of the most comprehensive and popular astrophysical reaction rate libraries. However, its experimentally obtained rates for light isotopes still rely mainly on the Caughlan and Fowler (1988) compilation and have never been updated despite the progress in many relevant nuclear astrophysics experiments. Moreover, due to fitting errors REACLIB is not reliable at temperatures lower than 10^7K. In this work we establish the formalism for updating the obsolete Caughlan–Fowler experimental rates of REACLIB. Then we use the NACRE compilation and results from the LUNA experiments to update some important charged-particle induced rates of REACLIB focusing on the proton–proton chain. The updated rates (available also in digital form) can now be used in the low temperature regime (below 10^7K) which was forbidden to the old version of REACLIB.

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1. Introduction

Nuclear reactions have long been established as the engines that provide the necessary energy for the stars which use that energy to balance the enormous gravitational pressure of the stellar gas (see Ref. [1] and references therein). Every stellar evolution code relies on a nuclear reaction rate library which is read by the code before any simulation is performed (see for example Refs. [2,3]. The size and accuracy of that library determine the quality of the relevant simulation and, therefore, its nuclear reaction rates should be continually improved and upgraded.

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One of the most comprehensive such libraries is REACLIB, updated [6] by the Basel nuclear astrophysics group and used extensively in small [5] and large [2] scale simulations. According to its authors, REACLIB cannot be safely used, due to fitting errors, at temperatures lower than $T_9 = 0.01$ (where T_9 measured in 10^9K) despite the fact that nuclear burning of hydrogen isotopes starts at lower temperatures, such as deuterium burning down the Hayashi line. That defect of REACLIB is an undesirable consequence of fitting a single formula to an array of data (see below) which spans many orders of magnitude (sometimes more than thirty!) with respect to a very extended temperature range $0.01 \leq T_9 \leq 10$. In fact even nuclear rates which are evaluated close to the upper limit of the critical temperature region are expected to be contaminated with similar (although less severe) fitting inaccuracies. For example, very important studies where the application of the old REACLIB rates may be questionable are pre-main and main-sequence stellar evolution simulations [3,5] including the solar evolution/neutrino studies where temperatures never exceed the value of $T_9 = 0.016$ (the central value of the present sun is roughly $T_9 = 0.0157$). Therefore, it is now obvious that all stellar evolution simulations which start from a Zero-Age Main Sequence star (ZAMS) are forced to apply REACLIB to temperatures well below $T_9 = 0.01$ yielding results which may be inaccurate.

According to the authors of REACLIB most of its charged-particle reaction rates for light nuclei rely on the compilation of Caughlan and Fowler [7]. However, since the publication of Ref. [7] there has been a very fertile activity in the field of experimental nuclear astrophysics leading to experiments which for the first time reached deep into the most effective energy of interaction of astrophysical reactions [8]. New reaction rate compilations have appeared either for light nuclei [9] or for heavier ones participating in explosive burning [10]. REACLIB has not yet been updated and its light nuclei experimentally-obtained rates are obsolete. Moreover, the Caughlan–Fowler [7] rates suffer from another source of inaccuracy since many higher energy resonances are lumped into one analytical term which is an undesirable oversimplification for plausible reasons.

According to a very relevant publication [11] computer programs have already been written which generate REACLIB parameters to fit the NACRE collaboration rates to within an accuracy of 2%. However, our group has written its own programs in the Mathematica computer language which yield very satisfactory results.

The present paper has three objectives:

(a) to use the NACRE compilation (as well as other more recent experimental data) in order to partially update the light-isotope experimental reaction rates of REACLIB. The update is focused on some of the most important reaction rates of the proton–proton chain which can now be used (in their updated version) in the critical temperature region $T_9 < 0.01$.

(b) to improve the REACLIB fitting accuracy in such a way which would allow its application to high quality studies related to the destruction of short-lived nuclei in pre-main sequence stellar evolution.

(c) to establish the formalism and techniques which will be used in future more extended updates of REACLIB.

The layout of the paper is as follows:

In Section 2 there is a brief description of the formalism used in the evaluation of light-nuclei thermonuclear reaction rates. In Section 3 the main components of REACLIB are presented while in Section 4 we describe the methodology adopted in order to accomplish the above mentioned objectives. In Section 5 some of the most important reactions of the proton–proton chain are updated, while the results of the present study are summarized in Section 6.

2. Calculation of thermonuclear reaction rates

The thermonuclear reaction rate (TRR) for the binary reaction $X(a,b)Y$ is given by the formula

$$r_{aX} = (1+\delta_{aX})^{-1} N_a N_X \langle \sigma u \rangle \,, \tag{1}$$

where N_a, N_X are the number densities and $\langle \sigma u \rangle$ stands for the reaction rate per pair of particles given by the formula:

$$\langle \sigma u \rangle = \sqrt{\frac{8}{\pi\mu}} \frac{1}{(kT)^{3/2}} \int\limits_0^\infty \sigma(E) E \exp\left(-\frac{E}{kT}\right) dE \,. \tag{2}$$

The Kronecker symbol δ_{aX} takes into account that the interacting nuclei can be identical.

The cross section $\sigma(E)$,which appears in the TRR, can be non-resonant (NR) or resonant according to the range of stellar energies E. If the temperature of the star is such that the integrand goes to zero before the cross section strikes a resonance, the non resonant formalism can be used by adopting the formula

$$\sigma(E) = \frac{S(E)}{E} e^{-2\pi\eta} \,, \tag{3}$$

where $S(E)$ is a slowly varying function of energy called the astrophysical factor and η is the usual Sommerfeld parameter defined as:

$$\eta = 0.1575 Z_1 Z_2 \left(\frac{A}{E}\right)^{1/2} . \tag{4}$$

The Z_1, Z_2 are the charge numbers of the interacting nuclei and A is the respective reduced mass number $A = A_1 A_2 (A_1 + A_2)^{-1}$ in a.m.u.

On the other hand if the most effective energy of interaction (see Eq. 7) is equal to the energy (E_r) of a quasi-stationary state of the ensuing compound nucleus then the cross section exhibits resonant behavior which can be described by the Breit–Wigner formula:

$$\sigma_\mathrm{r}(E) = \frac{\pi}{k^2}\omega \frac{\Gamma_i(E)\Gamma_f(E)}{(E-E_\mathrm{r})^2 + \Gamma(E)^2/4} , \tag{5}$$

where κ is the wave number, $\Gamma_i(E)$ and $\Gamma_f(E)$ are the entrance and exit channel partial widths, respectively, $\Gamma(E)$ is the total width, and ω is the statistical factor given by

$$\omega = (1 + \delta_{12}) \frac{(2J+1)}{(2J_1+1)(2J_2+1)} , \tag{6}$$

where J_1, J_2, J, are the spins of the interacting nuclei and of the resonance, respectively.

When the Breit–Wigner formula is inserted into Eq. (2) the integrand exhibits maxima at E_r and at the most effective energy of interaction E_0 given by

$$E_0 = 0.1220 (Z_1^2 Z_2^2 A)^{1/3} T_9^{2/3} \mathrm{MeV} . \tag{7}$$

The thermonuclear reaction rate (TRR) per pair of particles for an isolated narrow resonance E_r is given by [1]

$$\langle \sigma u \rangle_{E_\mathrm{r}} = \left(\frac{2\pi}{\mu k T}\right)^{3/2} \hbar^2 (\omega\gamma)_{E_\mathrm{r}} \exp\left(-\frac{E_\mathrm{r}}{kT}\right) , \tag{8}$$

where $(\omega\gamma)_{E_\mathrm{r}} = \omega \Gamma_i \Gamma_f / \Gamma(E_\mathrm{r})$.

For light nuclei which capture protons or alpha particles (such as those studied in the present paper) the compound nuclei will be produced at low excitation energies where the level densities are low. In such a case the statistical model (*i.e.* Hauser–Feshbach model) breaks down [10] and sometimes overestimates the reaction rates by several orders of magnitude. Therefore, the total Maxwellian averaged reaction rate $N_{\rm A}\langle\sigma u\rangle$ is determined by summing up the contributions of (i) single isolated (narrow) resonances

$$N_{\rm A}\langle\sigma u\rangle_{{\rm r}_i} = N_{\rm A}\left(\frac{2\pi}{\mu k}\right)^{3/2}\hbar^2(\omega\gamma)_{{\rm r}_i}T^{-3/2}\exp\left(-\frac{E_{{\rm r}_i}}{kT}\right) \tag{9}$$

and their single non-resonant (tail) contribution

$$N_{\rm A}\langle\sigma u\rangle_{\rm nr} = N_{\rm A}\left(\frac{2}{\mu}\right)^{1/2}\frac{\Delta E_0}{(kT)^{3/2}}S_{\rm eff}\exp\left(-\frac{3E_0}{kT}\right) \tag{10}$$

so that

$$N_{\rm A}\langle\sigma u\rangle = \sum_i N_{\rm A}\langle\sigma u\rangle_{{\rm r}_i} + N_{\rm A}\langle\sigma u\rangle_{\rm nr}\,. \tag{11}$$

In the latter expression we have used the familiar notation for rates used in many popular textbooks and articles such as Ref. [1] and Ref. [12]. The index (i) in Eq. (11) indicates a particular isolated resonance. Note that $S_{\rm eff}$ is the effective astrophysical factor which is given as a function of the experimentally derived zero-energy astrophysical factor and its derivatives $(S(0), S^{'}(0)\ldots)$ by the formula

$$S_{\rm eff}=S(0)\left[1+\frac{5}{12\tau}+\frac{S^{'}(0)}{S(0)}\left(E_0+\frac{35}{36}kT\right)+\frac{1}{2}\frac{S^{''}(0)}{S(0)}\left[E_0^2+\frac{89}{36}E_0kT\right]\right], \tag{12}$$

where the E_0 is the most effective energy of interaction, τ is given by $\tau = 4.248(Z_1Z_2AT_9)^{1/3}$ and A is the reduced mass number: $A = A_1A_2(A_1 + A_2)^{-1}$).

Nuclear astrophysics experiments measure all the components $(S(0), S^{'}(0)\ldots)$ of the effective astrophysical factor $S_{\rm eff}$, the resonance energies $E_{\rm r}$ and the respective partial widths. Those data are then inserted into Eq. (11) in order to provide formulas for the thermonuclear reaction rates which are used in stellar evolution simulations. However, thermonuclear reaction rate data are more easily used when they are given in tabular forms [6,9] so that they can be parameterized into reaction rate libraries by using suitable fitting formulas [4,6,10]. Those libraries are then uploaded directly by the simulation code for stellar evolution and nucleosynthesis calculations.

3. Brief description of REACLIB

REACLIB is a complete library of nuclear reaction rates. Using capital letters $A, B, C, \ldots$, to denote each isotope (parent and daughter ones) the reaction rate library REACLIB would consist of the following components:

DECAYS

Beta decays and electron captures: $A \longrightarrow B$

Photo-disintegration and beta delayed neutron emission: $A \longrightarrow B+C$

Inverse triple alpha or beta-delayed two neutron emission: $A \longrightarrow B+C+D$

BINARY REACTIONS

$A+B \longrightarrow C$

$A+B \longrightarrow C+D$

$A+B \longrightarrow C+D+E$

$A+B \longrightarrow C+D+E+F$

TRIPLE REACTION

$A+B+C \longrightarrow D$

$A+B+C \longrightarrow D+E$

Each rate is described by three lines. The first line indicates: (a) the participating nuclei, (b) the source of the reaction, (c) the type of reaction (resonant, non-resonant), (d) if the rate is calculated from the inverse reaction rate or not, (e) the Q value of the reaction in MeV. The second and third line for each rate give the seven fitting coefficients described below.

All reaction rates in REACLIB have been derived by using the seven-parametric ($a_i, i = 1 \ldots 7$) fitting formula

$$\begin{aligned} R_{\mathrm{tot}}(a_1 \ldots a_7; T_9) \;=\; & \exp(a_1 + a_2 T_9^{-1} + a_3 T_9^{-1/3} + a_4 T^{1/3} \\ & + a_5 T_9 + a_6 T_9^{5/3} + a_7 \ln T_9)\,, \end{aligned} \tag{13}$$

where the reaction rate $R_{\mathrm{tot}}(a_1 \ldots a_7; T_9)$ is measured in $\mathrm{cm^3 mol^{-1} s^{-1}}$ and corresponds to: $\ln 2/t_{1/2}$ for decays, $N_{\mathrm{A}}\langle ab\rangle$ for binary reactions, $N_{\mathrm{A}}^2\langle abc\rangle$ for triple-reactions (N_{A} being Avogadro's number), and T_9 is the temperature in units of GK. Actually, we have adopted the formalism of the original REACLIB library to avoid confusion. Note that the NACRE compilation uses the same definition for its rates (*i.e.* $\ln 2/t_{1/2}$, $N_{\mathrm{A}}\langle ab\rangle, N_{\mathrm{A}}^2\langle abc\rangle$). According to the above mentioned formalism (*i.e.* Eq. (9), Eq. (10), Eq. (11)) REACLIB splits the total charged-particle induced rate R_{tot} into one non-resonant $R_{\mathrm{nr}}(a_1^{\mathrm{nr}} \ldots a_7^{\mathrm{nr}})$ and (i) resonant components $R_{\mathrm{r}_i}(a_1^{\mathrm{r}_i} \ldots a_7^{\mathrm{r}_i})$ denoted, respectively by the superscripts (nr) and (r). Thus the total R_{tot} reaction rate will be

$$R_{\mathrm{tot}} = R_{\mathrm{nr}}(a_1^{\mathrm{nr}} \ldots a_7^{\mathrm{nr}}) + \sum_i R_{\mathrm{r}_i}(a_1^{\mathrm{r}_i} \ldots a_7^{\mathrm{r}_i})\,. \tag{14}$$

Note that one does not have to include all possible resonances of the compound nucleus which is formed during charged-particle capture reactions. It is sufficient to include those isolated (narrow) resonances which are relevant to the temperature (energy) regime where the rate will be applied to.

Regarding the use of REACLIB, stellar modelers often apply ([4,5], and references therein) REACLIB to the critical region $0.001 < T_9 < 0.01$ mentioned in our introduction, by using a very limited reaction network of light nuclei. Their decision is partly justified by the fact that at such low temperatures there is only a tiny nuclear energy production, while as regards nucleosynthesis only very light nuclei are destroyed such as deuterium, lithium *etc.* Sometimes nuclear burning at temperatures $T_9 < 0.0005$ is totally disregarded and only decays are considered. It is obvious that the obsolete Caughlan–Fowler [7] rates of REACLIB may have been a source of errors to all stellar evolution simulations [2–5] that have used it.

There are various versions of REACLIB which can be downloaded from Ref. [13].The most recent version of REACLIB currently available on-line [13] by the Basel group involves the unprecedented number of 5.411 isotopes with a mass numbers range $1 \leq A \leq 279$. However, its light-isotope charged-particle experimental rates are still those of Ref. [7], which underlines the importance of the present study.

4. Adopted methodology

Fitting the REACLIB formula Eq. (13) to the tabular reaction rate data (*e.g.* the NACRE ones) over the entire temperature range is not the most accurate approach. The fitting procedure is forced to fit a single formula to an array of data which spans many orders of magnitude (sometimes more than thirty!) with respect to a very extended temperature range $0.001 \leq T_9 \leq 10$. This approach generates, sometimes, a significant error which will be avoided in our study.

On the other hand, there are admittedly more sophisticated mathematical functions that could fit the data much better than Eq. (13), such as those given by NACRE [9]. However, we must follow the format of REACLIB otherwise we should be dealing with a different reaction rate library of a different format (whose fitting function might be taxing the computer considerably).

We must now turn to the format of the NACRE data which must be seriously taken into consideration. The NACRE data are given in the form of an array of values (rates with respect to temperature plus uncertainties) which is the result of combining various individual rate components, namely: non-resonant, narrow resonant + tails, broad resonant and multi-resonant rates. It is impossible to extract the individual rates from the combined NACRE tabular data although that is necessary in our work due to the format of REACLIB. Fortunately, the NACRE authors have also derived analytical approximations to each of these rate components, thus providing a tool for uploading the new NACRE rates into REACLIB. We use the

ORIGIN fitting package which relies on the Levenberg–Marquardt (LM) algorithm (one of the most powerful and reliable fitting methods) to perform non-linear regression. Actually, we fit Eq. (13) to each of these analytical approximations only over the temperature range where the respective rate component plays a non-negligible role to the total rate. Outside this range the new individual REACLIB rates may not be very reliable (although the total rate can be safely used). For example, if the non-resonant (NR) rate of a particular reaction is considerably smaller than the respective (first resonance) R1 rate at temperatures $T > T_9^*$ then our fitting range for the NR rate for that reaction would be $[0.001, T_9^*]$ provided the relevant NR Eq. (13) behaves asymptotically correctly at $T > T_9^*$ (*e.g.* it is a decreasing function of temperature). In such a case we would not recommend using individually the NR rate of that particular reaction at temperatures $T > T^*$. However, at $T < T_9^*$ that particular NR rate is suitable for all practical applications, where of course the relevant reaction rate obeys the general rule of Eq. (15).

Normally the fitting procedure would involve fitting Eq. (13) to the NACRE analytic functions. However, we have decided to fit the exponent of Eq. (13) to their natural logarithms, which is a more accurate approach.

As for the non-resonant rates of resonant reactions, we have calculated, in several cases the non-resonant rates by using the numerical integration formalism adopted by NACRE [9]. This was necessary in order to verify that the analytic formula given by NACRE has not been misprinted..

Note that in our fit we adopt the assumption made by NACRE [9] that all rates $N_{\rm A}\langle\sigma u\rangle$ which obey the condition

$$N_{\rm A}\langle\sigma u\rangle \leq 10^{-25} \tag{15}$$

can be considered negligible in practically all astrophysical applications.

We assess the quality and relevance of the updated REACLIB by using the following three tools:

Firstly, we can ascertain that the new (updated) total REACLIB rates approximate satisfactorily the total NACRE ones by plotting their relative difference RD with respect to temperature (T_9) using:

$$\mathrm{RD}(T_9) = 100\, \frac{R_{\rm tot}^{\rm REACLIB(new)}(T_9) - R_{\rm tot}^{\rm NACRE}(T_9)}{R_{\rm tot}^{\rm REACLIB(new)}(T_9)}\%\,. \tag{16}$$

Secondly, we can assess the relevance of updating the REACLIB rates (*i.e.* the present work) by plotting the variation of the relative difference between the old total REACLIB rate and the total NACRE rates, with respect to temperature (T_9) by using:

$$\mathrm{RD}(T_9) = 100\, \frac{R_{\rm tot}^{\rm REACLIB(old)}(T_9) - R_{\rm tot}^{\rm NACRE}(T_9)}{R_{\rm tot}^{\rm REACLIB(old)}(T_9)}\%\,. \tag{17}$$

Thirdly we can assess the deviation between the new and the old REACLIB rates by plotting their relative difference with respect to time. Provided that the new REACLIB rates approximate well the NACRE ones this tool is also a measure of the relevance of the present update:

$$\mathrm{RD}(T_9) = 100\,\frac{R_{\mathrm{tot}}^{\mathrm{REACLIB(old)}}(T_9) - R_{\mathrm{tot}}^{\mathrm{REACLIB(new)}}(T_9)}{R_{\mathrm{tot}}^{\mathrm{REACLIB(old)}}(T_9)}\,\%\,. \tag{18}$$

When necessary, we plot the variation of RD (%) with respect to temperature for two different temperature regimes: The first regime is relevant to solar evolution simulations while the second one covers the entire temperature range given by NACRE.

In each figure caption we also include the accuracy ($n\%$) of the analytical approximation given by NACRE (see Appendix B of Ref. [9]). Therefore, all the updated REACLIB reaction rates relying on the NACRE compilation carry an inherent fitting error of ($n\%$).

5. Updating the reactions of the proton–proton chain

5.1. Reaction $^1H(p,\nu e^+)^2H$

This reaction is of paramount importance to stellar evolution and especially to solar evolution and neutrino solar studies. Therefore, its thermonuclear reaction rate at relevant temperatures should be as accurate as possible.

Adopting the same formula for the astrophysical factor as the one given by NACRE [9]:

$$S(E) = 3.94 \times 10^{-25} \times (1 + 11.7E + 75E^2)\,\mathrm{MeV\,b}$$

we numerically integrate Eq. (2) and then fit Eq. (13) to the derived tabular data over the region $0.001 < T_9 < 0.1$. We confined our fit to a much shorter range $0.001 < T_9 < 0.02$ but the accuracy did not improve. It is obvious from Fig. 1 that at temperatures $T_9 < 0.1$ the old REACLIB values are very close to the new ones, therefore the old $^1\mathrm{H}(p,\nu e^+)^2\mathrm{H}$ rate need not be updated as regards the solar evolution zone. Although at temperatures $T_9 < 0.1$ both the old and the new REACLIB rates approximate well the NACRE data, at higher temperatures the old REACLIB rate significantly deviates from the NACRE one. This deviation is particularly relevant to explosive hydrogen burning simulations which sometimes are performed using the REACLIB library (*e.g.* the TYCHO [4] code, which is based on the REACLIB library, is equipped with explosive burning simulation engines). Therefore, we recommend the use of the present updated reaction rate parameters over the entire spectrum of temperatures: $0.001 < T_9 < 10$.

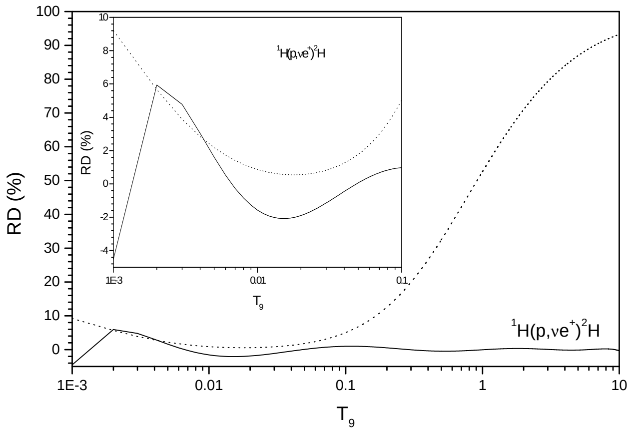

Fig. 1. ^{1}H$(p, \nu e^+)^2$H: The variation RD(%) of the relative difference between the REACLIB rates and the values obtained by numerical integration of Eq. (2) using the NACRE data. The solid curve represents the RD between the new REACLIB rate and the NACRE one while the dotted one represents the RD between the old REACLIB rate and the NACRE one ($n = 3\%$).

5.2. Reaction $^2H(p, \gamma)^3He$

NACRE specifies two temperature regimes and fits two different functions for the reaction rates. However, REACLIB cannot follow the same format. Instead, we fitted the REACLIB rate formula to the NACRE tabulated rates and we found that the NACRE rates and those given by the new REACLIB are almost identical for the entire low-temperature regime.

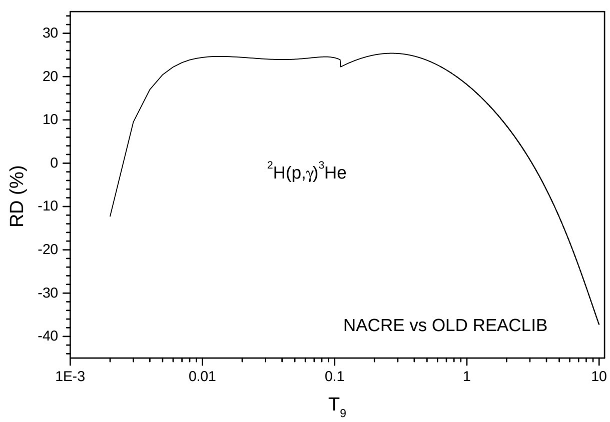

Fig. 2. ^{2}H$(p, \gamma)^3$He: The variation of the relative difference RD between the old REACLIB rates and the NACRE ones with respect to temperature ($n = 3\%$).

However, we observe a 37% maximum relative difference between the old REACLIB rates and the NACRE ones while at the solar temperature regime, in particular, the RD is roughly 25%. All deuterium burning studies which have relied on the old REACLIB should take this observation seriously into account.

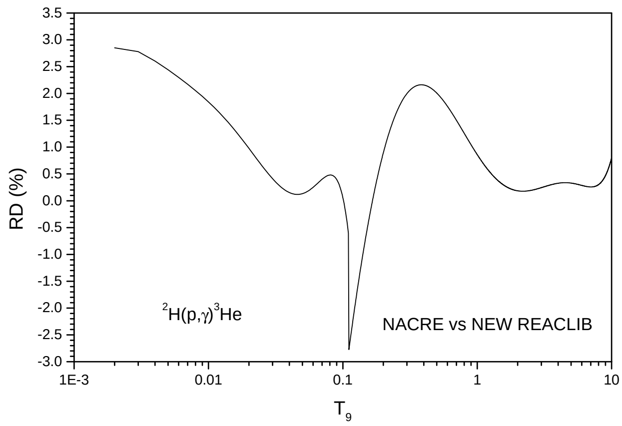

Fig. 3. ^{2}H$(p,\gamma)^3$He: The variation of the relative difference RD between the new REACLIB rates and the NACRE ones with respect to temperature ($n = 3\%$).

5.3. Reaction $^2H(d,\gamma)^4He$

Fitting the REACLIB formula (*i.e.* Eq. (13) to the tabulated data of the NACRE compilation yields very satisfactory results. The new REACLIB formula fits excellently the NACRE tabular data and, therefore, plotting the variation of the relevant RD with respect to temperature is unnecessary. Instead, we plot the variation of the relative difference between the old and the new REACLIB rates with respect to temperature. Figure 4 shows that the old REACLIB rate in the solar temperature-regime can be up to 15% larger than the rate predicted by NACRE while this discrepancy is fixed by the new fit. The updated REACLIB rate is practically the same as the NACRE one in the same regime. However, as shown in the same figure, at larger temperatures the new REACLIB rate (*i.e.* the NACRE rates) are significantly larger than the old ones.

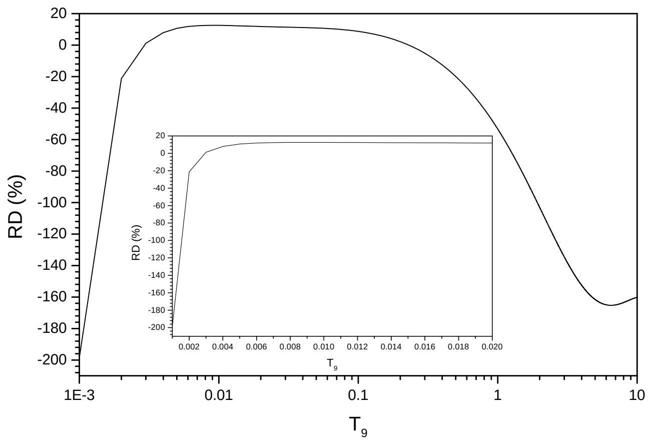

Fig. 4. ^{2}H$(d,\gamma)^4$He: The variation of the relative difference RD between the new and old REACLIB rates with respect to temperature ($n = 3\%$).

5.4. *Reaction* $^2H(d,n)^3He$

The new REACLIB formula fits excellently the NACRE tabular data and thus, as in the case of ^{2}H$(d,\gamma)^4$He reaction we only plot the variation of the relative difference between the old and the new REACLIB rates with respect to temperature.

According to Fig. 5 in the solar regime the old REACLIB rates are up to 12% smaller than the new (or NACRE) ones while at higher temperatures this effect is reversed and the old rates become larger than the new ones (up to 90%).

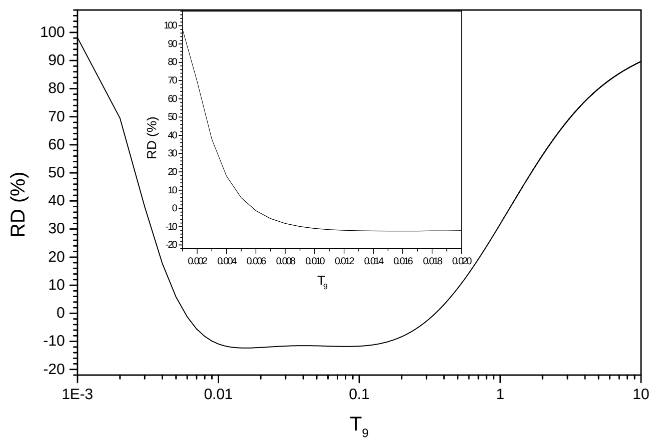

Fig. 5. ^{2}H$(d,n)^3$He: The variation of the relative difference RD between the new and old REACLIB rates with respect to temperature ($n = 4\%$).

5.5. Reaction $^2H(d,p)^3H$

The new REACLIB formula fits excellently the NACRE tabular data. According to Fig. 6 in the solar regime the old REACLIB rates are up to 10% smaller than the new (or NACRE) ones while at higher temperatures this effect is reversed and the old rates become larger than the new ones (up to 90%).

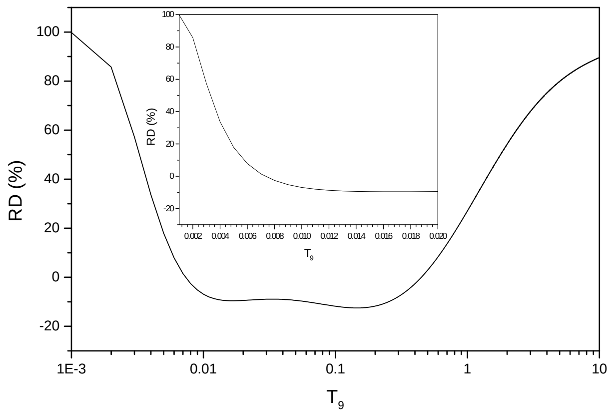

Fig. 6. ^{2}H$(d,p)^3$H: The variation of the relative difference RD between the new and the old REACLIB rates with respect to temperature ($n = 5\%$).

5.6. Reaction $^3He(^3He,2p)^4He$

For this reaction we do not rely on NACRE data in order to produce its REACLIB rate. The LUNA collaboration has managed recently to lower the beam energy of their experiment so much that they have evaluated the relevant astrophysical factor with the highest precision ever. Therefore, we follow the most reliable procedure of numerically integrating the thermonuclear reaction rate integral, a method followed by NACRE as well.

Then we fit Eq. (13) to the array of numerical data. The new REACLIB formula represents the data very satisfactorily and according to Fig. 7 there is a notable deviation from the old REACLIB formula, which may have a non-negligible effect on solar evolution simulations using REACLIB.

In Fig. 7 we plot the variation of the RD between the REACLIB rates (old and new) and the rate obtained by numerically integrating Eq. (2) using the most recent LUNA data. We observe that the RD between the new REACLIB and the LUNA rates (solid curve) is consistently smaller than the respective RD (dotted curve) between the old REACLIB and the LUNA rates. Especially in the solar regime the old REACLIB rate deviates from the LUNA one by up to 7% whereas, in the same temperature-region, the RD between the new REACLIB rate and the LUNA one is less than 1%.

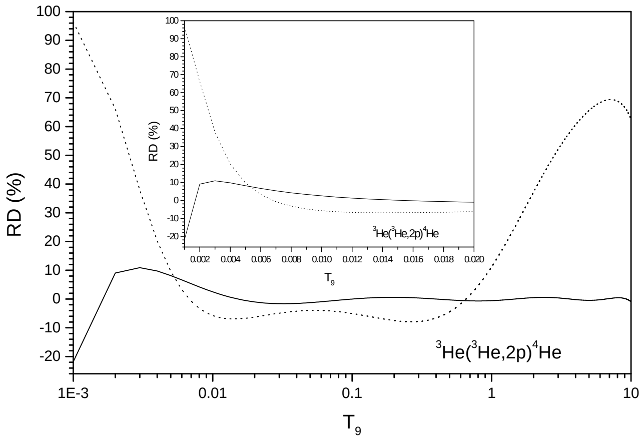

Fig. 7. ^{3}He(^{3}He$, 2p)^4$He: The variation of the relative difference RD between the (old/new) REACLIB rates and that obtained by using the LUNA data with respect to temperature. The solid (dotted) curve represents the RD between the new (old) REACLIB rate and the LUNA one.

5.7. Reaction $^3He(\alpha,\gamma)^7Be$

The new REACLIB formula fits excellently the NACRE tabular data. According to Fig. 8 in the solar region the new REACLIB rate approximates the NACRE rate with an accuracy of 1% or better, while the old

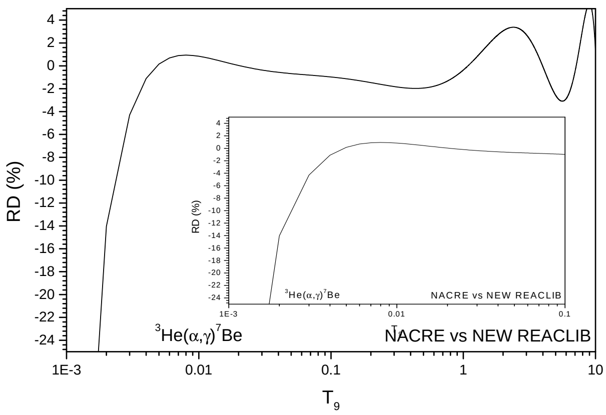

Fig. 8. ^{3}He$(\alpha,\gamma)^7$Be: The variation of the RD between the new REACLIB rate and the NACRE one with respect to temperature ($n = 6\%$).

REACLIB rate (see Fig. 9) can be up to 2.5% larger than the NACRE one. According to Fig. 10, which shows the deviation between the old and the new REACLIB rates, the new REACLIB rate is approximately the same as the old REACLIB one. However, due to the importance of the ^{3}He$(\alpha,\gamma)^7$Be reaction in the solar neutrino studies we recommend using the new updated REACLIB rate.

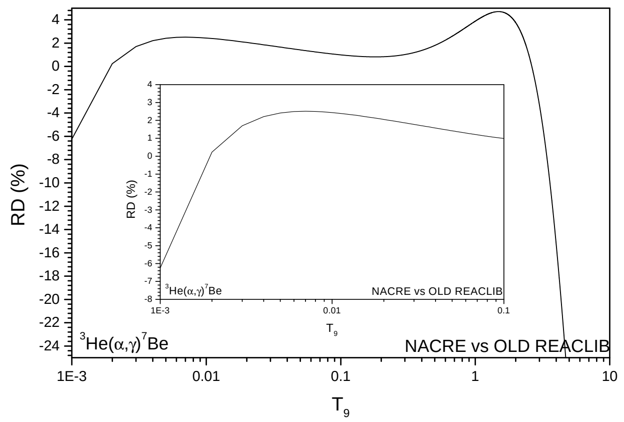

Fig. 9. ^{3}He$(\alpha,\gamma)^7$Be: The variation of the RD between the old REACLIB rate and the NACRE one with respect to temperature ($n = 6\%$).

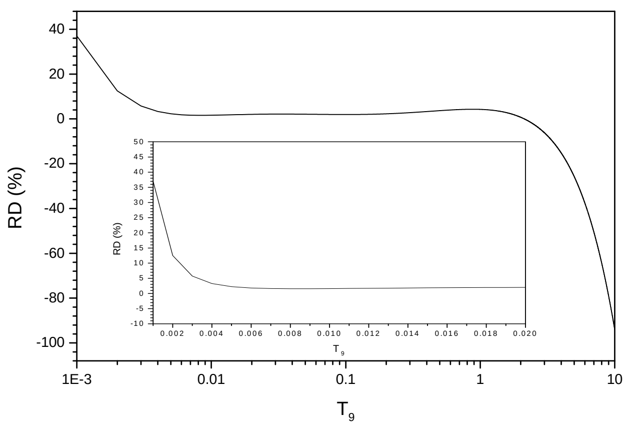

Fig. 10. ^{3}He$(\alpha,\gamma)^7$Be: The variation of the RD between the old and the new REACLIB rates with respect to temperature ($n = 6\%$).

5.8. Reaction $^6Li(p,\gamma)^7Be$

The new REACLIB rate approximates much better the NACRE rate than the old one. According to Figs. 11 and 12 in the solar region the old REACLIB rate can differ from the NACRE rate by up to 80% while the respective discrepancy for the new REACLIB is always less than 2%.

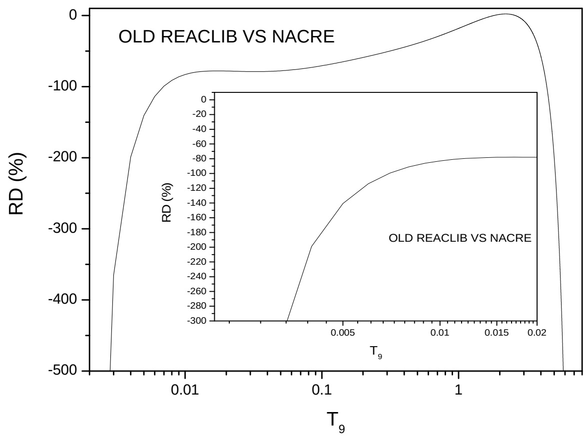

Fig. 11. ^{6}Li$(p,\gamma)^7$Be: The variation of the RD between the old REACLIB rate and the NACRE one with respect to temperature ($n = 7\%$).

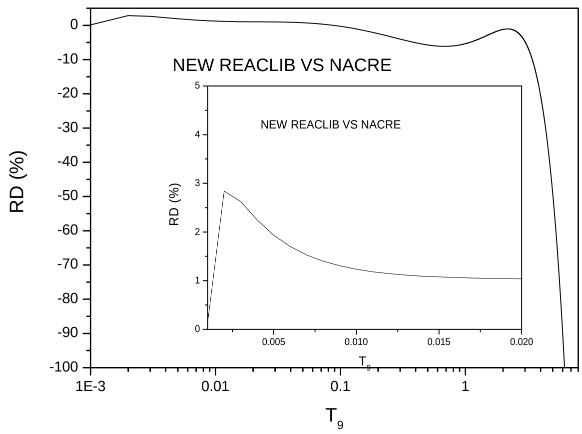

Fig. 12. ^{6}Li$(p,\gamma)^7$Be: The variation of the RD between the new REACLIB rate and the NACRE one with respect to temperature ($n = 7\%$).

5.9. Reaction $^6Li(p,\alpha)^3He$

REACLIB distinguishes two components for that rate: a non-resonant and a resonant one while NACRE adopts a single non-resonant fit. By fitting Eq. (13) to the single analytic formula given by NACRE we observe a very satisfactory representation of all the NACRE tabulated data. In Fig. 13 we compare the new REACLIB fit and the old two-component one where a minor deviation between the new fit and old one is observed. Accordingly we recommend a single non-resonant REACLIB formula for the updated library.

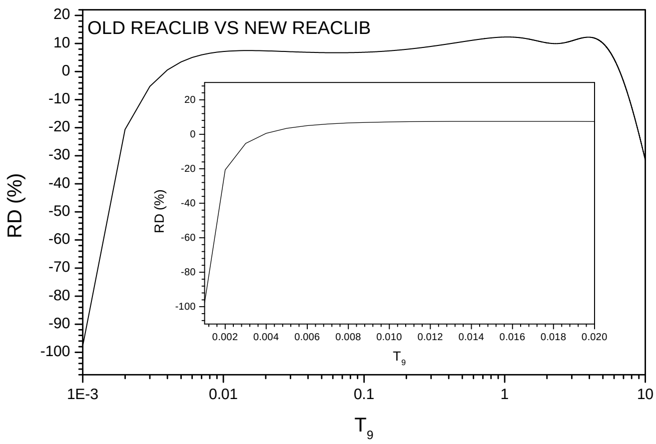

Fig. 13. ^{6}Li$(p,\alpha)^3$He: The variation of the RD between the old REACLIB rate and the new one with respect to temperature (2%).

5.10. Reaction $^7Li(p,\gamma)^8Be$

This reaction is missing from REACLIB and so is the relevant ensuing decay ^{8}Be$\rightarrow^4$He+^{4}He, we cannot therefore compare the new REACLIB rates to the old ones. The importance of this reaction to the PPII chain is that it is in competition with the ^{7}Li$(p,\alpha)^4$He reaction, the latter being much more important to the solar evolution studies. The ^{8}Be produced in the ^{7}Li$(p,\gamma)^8$Be reaction, which is unstable and decays into two alpha particles in 2.6×10^{-16}s, is extremely important to the triple alpha reaction as well. Due to the importance of that reaction we will defer its study (and/or update) to a later paper where we will also investigate the effects of its absence on the simulations that have used REACLIB.

5.11. Reaction $^7Li(p,\alpha)^4He$

According to Fig. 14 the non-resonant rate dominates at temperatures $T_9 < 4$. We have compared the NACRE rates and those given by the old REACLIB and have found that their small differences are within the relevant uncertainties. Therefore, no update was deemed necessary for that reaction.

5.12. Reaction $^7Li(\alpha,\gamma)^{11}B$

NACRE evaluates the rates using a non-resonant (NR), a resonant (R1) and a multi-resonant (MR) rate (see Fig. 15) while REACLIB relies only on a NR and a R1 rate. In Fig. 16 we plot the variation of RD between the old/new REACLIB rates and the NACRE one for all relevant temperatures.

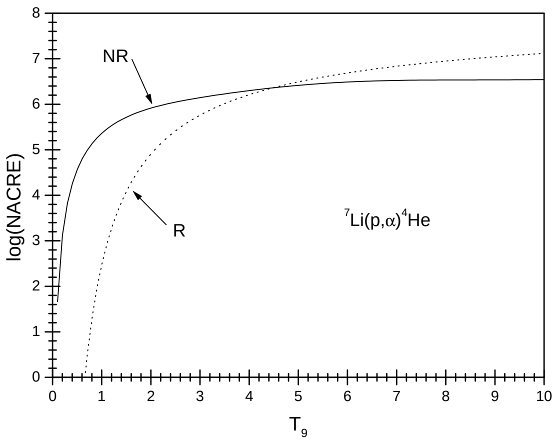

Fig. 14. $^7\mathrm{Li}(p,\alpha)^4\mathrm{He}$: The logarithms of the NACRE rates (resonant and non-resonant) with respect to temperature (6%).

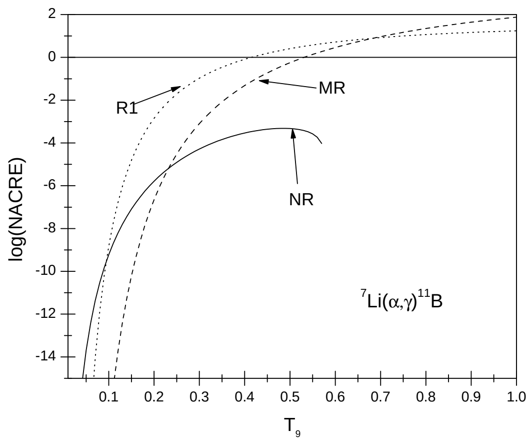

Fig. 15. $^7\mathrm{Li}(\alpha,\gamma)^{11}\mathrm{B}$: The logarithms of the NACRE rates (resonant, non-resonant and multiresonant) with respect to temperature ($n = 17\%$).

We do not include an inset figure for the solar regime as that particular reaction is irrelevant to solar evolution studies. It is obvious that the updated rates approximate the NACRE ones better than the old REACLIB ones.

5.13. Reaction $^7Be(p,\gamma)^8B$

The NACRE non-resonant data for this reaction have been superseded by more recent ones [14]. According to NACRE [9], the recommended S-factor at zero energy is $S_{17}(0) = 21 \pm 2\,\mathrm{eV\,b}$, while according to Ref. [14] it should be $S_{17}(0) = 18.6 \pm 1.2\,\mathrm{eV\,b}$. Despite the notable difference in the zero-energy astrophysical factor we decided to use the NACRE data for con-

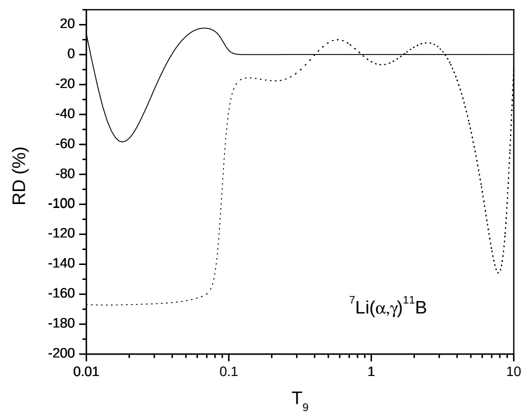

Fig. 16. ^{7}Li$(\alpha, \gamma)^{11}$B: The variation of the RD between the old (solid curve)/ new(dotted curve) REACLIB rates and the NACRE one with respect to temperature ($n = 17\%$).

sistency. However, it should be noted that for high quality solar neutrino calculations the more recent value [14] should be adopted which would lead to an 11.4% decrease in the relevant non-resonant rate.

The new REACLIB fitting approximates the NACRE tabular data better than the old one in the range $0.002 < T_9 < 2.2$ while at higher temperatures the old REACLIB rate constitutes a better approximation. Due to the large uncertainties involved at such high temperatures, we recommend the use of the updated REACLIB rates over the entire spectrum of temperatures. In Fig. 17 we observe that the NR component of the rate dominates the R1

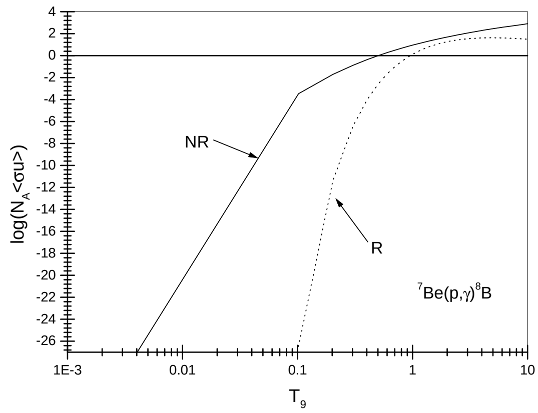

Fig. 17. ^{7}Be$(p, \gamma)^8$B: The logarithms of the NACRE rates (resonant, non-resonant and multiresonant) with respect to temperature ($n = 3\%$).

one everywhere. In Fig. 18 we plot: (a) the variation of the RD between the new REACLIB rate and the NACRE one (solid curve) and (b): the variation of the RD between the old and the new REACLIB rates (dotted curve). It is obvious that the new REACLIB rates are generally more reliable than the old ones especially at the solar evolution regime.

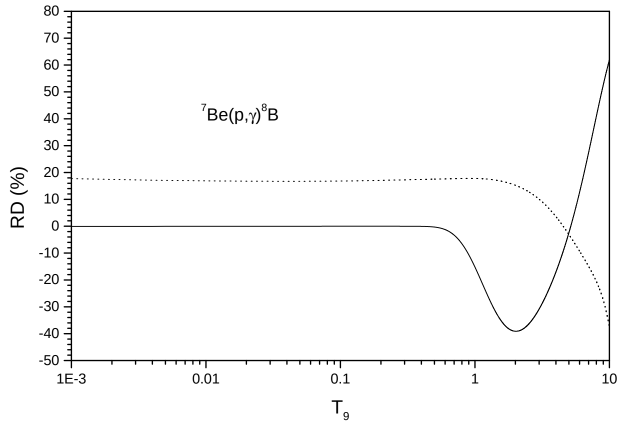

Fig. 18. $^{7}\mathrm{Be}(p,\gamma)^{8}\mathrm{B}$: The variation of the RD between the new REACLIB rate and the NACRE one (solid curve) and the variation of the RD between the old and the new REACLIB rates (dotted curve) ($n = 3\%$).

6. Summary and conclusions

The REACLIB is one of the most comprehensive and popular nuclear reaction rate library and it is extensively used in stellar evolution and nucleosynthesis simulations. In the present study, some very important light-isotope charged-particle experimental rates of REACLIB have been updated using the NACRE compilation [9] and results from the LUNA experiments [8]. We have focused on the reaction rates most important of the proton–proton chain reactions which are the most important thermonuclear processes occurring in the interior of the sun. The updated REACLIB rates can be used at temperatures which were forbidden in the old version. The deviation between the new and the old REACLIB rates is sometimes significant, especially at the low temperature regime ($0.001 < T_9 < 0.01$) of deuterium burning $^{2}\mathrm{H}(d,\gamma)^{4}\mathrm{He}$, $^{2}\mathrm{H}(d,p)^{3}\mathrm{H}$, $^{2}\mathrm{H}(d,n)^{3}\mathrm{He}$, where the old REACLIB rates were unreliable. Another notable rate-deviation is that the most important reaction $^{1}\mathrm{H}(p,\nu e^{+})^{2}\mathrm{H}$ appears to be faster in the updated REACLIB than in the old one. The effects of these deviations on explosive hydrogen burning and big-bang nucleosynthesis should be carefully investigated by adopting successively, the old and the new REACLIB libraries in relevant simulations (currently under study by the authors).

Another improvement of the new REACLIB rates (which are also available in the same digital form like the old ones) is that we have improved their fitting accuracy in such a way which allows their application to pre-main sequence stellar evolution, *i.e.* to the stars which are in the pro zero-age epoch before the hydrogen burning start. Finally we have established the formalism and techniques which will be used in future more extended updates of REACLIB (soon to appear by the authors).

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