The triple alpha reaction rate and the $2^+$ resonances in $^{12}\text{C}$

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The triple alpha rate is obtained from the three-body bound and continuum states computed in a large box. The results from this genuine full three-body calculation are compared with standard reference rates obtained by two sequential two-body processes. The fairly good agreement relies on two different assumptions about the lowest $2^+$ resonance energy. With the same $2^+$ energy the rates from the full three-body calculation are smaller than those of the standard reference. We discuss the rate dependence on the experimentally unknown $2^+$ energy. Substantial deviations from previous results appear for temperatures above 3 GK.

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Introduction. The triple alpha process is the key reaction that permits to bridge the $A = 5$ and $A = 8$ gaps, opening the door to the production of $^{12}\text{C}$ in the core of the stars in the red giant phase [4].

The properties of the $\alpha-\alpha-\alpha$ continuum states are crucial for the reaction rates, which determine the abundance of $^{12}\text{C}$ in the Universe. As a clear example, this is what led Fred Hoyle to predict the existence of a $0^+$ resonance just above the triple $\alpha$ threshold [2]. It is not possible to explain the observed abundance of $^{12}\text{C}$ without this so called Hoyle state, which was confirmed experimentally [3] to be at an energy of 0.38 MeV above the three-body threshold. The Hoyle state enhances by itself the reaction rate by about two orders of magnitude at low temperatures (below 2 GK), where the rate is dominated by the electric quadrupole transition from continuum $3\alpha$ $0^+$ states to the excited bound $2^+$ state in $^{12}\text{C}$.

In type-II supernova explosions dense and hot environments are created. This is the so called hot bubble, consisting of alpha-particles and neutrons, with rather uncertain but relatively high temperature reaching several GK [4]. These environments are the suggested place for the rapid-neutron process [5]. Although the importance of the triple alpha contribution as compared to other reactions in this temperature range ($T \gtrsim 2$ GK) has been questioned [6], it has also been suggested that changes in the reaction rate imply changes in estimates of the relative amounts of elements formed during the supernova explosion, and therefore in estimates of the rate at which heavy elements are distributed through the Universe [7].

In [8] the estimated reaction rate for the triple alpha reaction in this temperature range was found to be about an order of magnitude lower than the one given in [3], which would lead to a mass fraction of $^{56}\text{Ni}$ about two to three times smaller. At temperatures above 3 GK, the reaction rate for the triple alpha reaction is dominated by the electric quadrupole $2^+ \rightarrow 0^+_1$ transition [9] (we follow the notation where $J_i^\gamma$ represents the $i^{th}$ state in the spectrum with angular momentum $J$ and parity $\pi$). In the particular case of $^{12}\text{C}$ the states $0^+_1$ and $2^+_1$ are the only ones bound). The reaction rate in this region is therefore to a large extent determined by the properties of the $2^+$ continuum states, and in particular by the possible existence of a $2^+_2$ resonance at a relatively low energy. The properties of such a state is still an open problem. The reaction rates given in [8, 10] were computed assuming that $^{12}\text{C}$ has a $2^+_2$ resonance at 1.75 MeV. However, in [8] no evidence was found concerning the existence of such $2^+$ resonance. On the contrary, in [11] an experimental energy of about 2.3 MeV is derived. This value is substantially higher than the one used in [8, 10], and it could substantially modify their computed results. Also, in [12], where a three-body calculation is employed to obtain the resonances as poles of the $S$-matrix, a $2^+_2$ resonance has been found at an energy of 1.38 MeV. However, this energy is found with the same (adjustable) three-body interaction that reproduces the energy of the bound $2^+_1$ state.

The role of the $2^+_2$ resonance in $^{12}\text{C}$ in the triple alpha reaction rate requires detailed investigation. We shall employ the same three-body method as in [13], where no assumption is made about the capture mechanism (sequential or direct), and in contrast to the method described in [9], where a sequential capture process is assumed. The standard procedure and the almost canonical results of [9] is furthermore tested by comparison.

Full three-body formulation. The first of the methods used in this work is the three-body calculation described in [13]. Let us consider the radiative capture process $a + b + c \rightarrow A + \gamma$, where $A$ is a bound system made of particles $a$, $b$, and $c$ with separation energy $B_A$. The corresponding reaction rate $R_{abc}(E)$ is given by [13, 14]

$$ R_{abc}(E) = \frac{\hbar^3}{c^2} \frac{8\pi}{(\mu_{ab}g_{\gamma})^{3/2}} \left( \frac{E_{\gamma}}{E} \right)^2 \frac{2g_A}{g_{\gamma}g_{b\gamma}} \sigma_\gamma(E_{\gamma}) $$

where $E = E_{\gamma} + B_A$ is the initial three-body kinetic energy, $E_{\gamma}$ is the photon energy, $\sigma_\gamma(E_{\gamma})$ is the photo dissociation cross section of the $A$ nucleus, $c$ is the velocity of light, $g_i$ is the spin degeneracy of states of particle
i = a, b, c, A, and μx and μy are the reduced masses of the systems related to the Jacobi coordinates, (x, y), for the three-body system[13].

The photo dissociation cross section for the inverse process A + γ → a + b + c can be expanded into electric and magnetic multipoles. In particular, the electric multipole contribution of order λ has the form[13]:

\[ \sigma_\gamma^{(\lambda)}(E_\gamma) = \frac{(2\pi)^3(\lambda + 1)}{\lambda!(2\lambda + 1)!!} \left( \frac{E_\gamma}{\hbar c} \right)^{2\lambda-1} dB \frac{d\sigma}{dE}, \]

where the strength function B is

\[ B(E\lambda, n_0 J_0 \rightarrow nJ) = \sum_{\mu M} \left| (nJM)|O_\mu^\lambda|^2 \right|^2, \]

where \( J_0 \), J and \( M_0, M \) are the total angular momenta and their projections of the initial and final states, and all other quantum numbers are collected into \( n_0 \) and \( n \). The electric multipole operator is given by:

\[ O_\mu^\lambda = \sum_{i=1}^3 z_i |r_i - R|^3 Y_{\lambda \mu}(\Omega_{yi}) \]

where \( i \) runs over the three particles of charges \( z_i \), and where we neglect contributions from intrinsic transitions within each of the three constituents[16].

Finally the energy averaged reaction rate is obtained as a function of the temperature by using the Maxwell-Boltzmann distribution as weighting function. For three alpha particles we obtain[13]:

\[ \langle R_{\alpha\alpha\alpha}(E) \rangle = \frac{\hbar^3}{c^2 (\mu_{\alpha\alpha}\mu_{\alpha\alpha})^{3/2}} (2J + 1)e^{-\frac{E}{kT}} \times \]

\[ \left| (nJM)|O_\mu^\lambda|^2 \right|^2 \int_{|B|}^\infty E_\gamma^2 \sigma_\gamma^{(\lambda)}(E_\gamma)e^{-\frac{E_\gamma}{\pi\hbar^2}} dE_\gamma, \]

where \( k_B \) is the Boltzmann constant.

The strength function B is computed by genuine three-body calculations of both the bound final state, \( |n_0 J_0 M_0 \rangle \), and the continuum initial states, \( |nJM \rangle \). We use the hyperspherical adiabatic expansion method described in[15]. The \( \alpha-\alpha \) interaction is given in[17]. The basic procedure is computation of three-body states of given angular momentum and parity confined by box boundary conditions[18]. In this way the continuum spectrum is discretized. The strength functions are then obtained for each discrete continuum state according to Eq.[15]. The distribution \( dB/dE \) is built by use of the finite energy interval approximation, where the energy range is divided into bins, and all the discrete values of B falling into a given bin are added. Afterwards the points are connected by spline operations and the expressions[20] and[21] are computed.

**Sequential process.** The NACRE results given in[9] are usually taken as the reference for the reaction rates in the triple alpha process. In this work the process is assumed to proceed in a sequentially two-step process.

In the first step one \( \alpha \)-particle captures another one to produce \(^8\text{Be}\) in the ground \( 0^+ \) resonant state. In the second step, \(^8\text{Be}\) is able to capture (before decaying) a third \( \alpha \)-particle, populate a \(^{12}\text{C}\) resonance, and then decay by photo emission to one of the bound states of \(^{12}\text{C}\). The reaction rate for such a two-step process is given by the rate for the capture of an \( \alpha \)-particle by \(^8\text{Be}\) \((\langle R_{\alpha\alpha\alpha}(E''', E''') \rangle)\) weighted with the rate for formation of \(^8\text{Be}\)[8]:

\[ \langle R_{\alpha\alpha\alpha}(E''') \rangle = \frac{3\pi \hbar}{\mu_{\alpha\alpha}} \left( \frac{\mu_{\alpha\alpha}}{2\pi k_B T} \right)^{3/2} \int_0^{\infty} \sigma_{\alpha\alpha}(E'') e^{-\frac{E''}{k_B T}} \langle R_{\alpha\alpha\alpha}(E'', E''') \rangle dE''', \]

where \( E'' \) and \( E' \) are the relative energy between the two \( \alpha \)-particles forming \(^8\text{Be}\) and the energy of the third \( \alpha \)-particle relative to the center of mass of the first two, respectively. The temperature is \( T \) and \( \mu_{\alpha\alpha} \) is the reduced mass of the two-alpha system. The elastic \( \alpha-\alpha \) cross section is given by:

\[ \sigma_{\alpha\alpha}(E'') = \frac{2\pi}{\kappa^2} \Gamma_{\alpha}(^{8}\text{Be}, E'')^2 \int_{|B|}^\infty \sigma_{\alpha\alpha}(E''') e^{-\frac{E'''}{\pi\hbar^2}} dE''', \]

where \( \kappa^2 = 2\mu_{\alpha\alpha} E''/\hbar^2 \), \( E_r \) is the \(^8\text{Be}\) resonance energy, and the width \( \Gamma_{\alpha}(^{8}\text{Be}, E'') \) has the form[9]:

\[ \Gamma_{\alpha}(^{8}\text{Be}, E'') = \frac{P_r(E'')}{P_r(E_r)}, \]

where \( \Gamma_{\alpha} \) is the width of the resonance, \( P_r \) is the penetration factor, and \( \ell \) is the relative orbital angular momentum between the two \( \alpha \)-particles.

In our case, the experimental energy of the \( 0^+ \) resonance in \(^8\text{Be}\) is \( E_r = 0.09189 \text{ MeV} \) above threshold, with a width of \( \Gamma_{\alpha} = 6.8 \pm 1.7 \cdot 10^{-6} \text{ MeV} \). For such a narrow resonance we have that \( \Gamma_{\alpha}(^{8}\text{Be}, E'') \approx \Gamma_{\alpha}, \) and for our purpose we can safely replace Eq.[17] by:

\[ \frac{\sigma_{\alpha\alpha}(E'')}{\Gamma_{\alpha}(^{8}\text{Be}, E'')} = \frac{4\pi^2}{\kappa^2} \delta(E'' - E_r), \]

from which Eq.[16] becomes:

\[ \langle R_{\alpha\alpha\alpha}(E''') \rangle = \frac{3\pi \hbar}{\mu_{\alpha\alpha}} \left( \frac{\mu_{\alpha\alpha}}{2\pi k_B T} \right)^{3/2} \times \int_{|B|}^\infty \sigma_{\alpha\alpha}(E''') e^{-\frac{E'''}{\pi\hbar^2}} dE''', \]

Finally, from Ref.[9] we have:

\[ \langle R_{\alpha\alpha\alpha}(E''') \rangle = \frac{8\pi}{\mu_{\alpha\alpha}^2} \left( \frac{\mu_{\alpha\alpha}}{2\pi k_B T} \right)^{3/2} \times \int_0^{\infty} \sigma_{\alpha\alpha\alpha}(E'') e^{-\frac{E''}{k_B T}} E' dE'', \]

where

\[ \sigma_{\alpha\alpha\alpha}(E'') = \sum_{J=0,2} (2J + 1) \frac{\pi \hbar^2}{2\mu_{\alpha\alpha}^2 E_r} \frac{\Gamma_{\alpha}(^{12}\text{C}', E') \Gamma_{\alpha}(^{12}\text{C}', E'')}{(E_r - E''')^2 + 0.25(z^{12}\text{C}', E'')^2} \]
\[ E_r^J \] is the \( ^{12}\text{C} \) resonance energy with angular momentum \( J \), and
\[
\Gamma^{(12C^J, E')} = \Gamma_\alpha^{(12C^J, E')} + \Gamma_\gamma^{(12C^J, E')} \quad (13)
\]
\[
\Gamma_\alpha^{(12C^J, E')} = \frac{\Gamma_\alpha^{(12C^J)} P(E')} {P_r(E_r^J)} \quad (14)
\]
\[
\Gamma_\gamma^{(12C^J, E')} = \frac{\Gamma_\gamma^{(12C^J)} (E_r^J + E')^5} {E_r^J + E' + \Gamma_\gamma^{(12C^J, E')}^5} \quad (15)
\]

The parameters needed to compute Eq. (12), and therefore (11) and (10), are taken from [9] and they are collected in Table I.

Given a transition between \( ^{12}\text{C} \) continuum states with angular momentum \( J \) and a bound \( ^{12}\text{C} \) state with binding energy \( B_J \), it is now possible to extract the expression for \( dB/\text{d}E \) effectively used in Ref. [9]. This can be made by inserting Eq. (11) into (10), and Eq. (2) with \( \lambda=2 \) into Eq. (9). By comparison of those expressions we extract:
\[
dB \big/ \text{d}E = \frac{1}{\alpha} \frac{375 (hc)^4} {8 \pi^2 (E + |B_J|)^5} \frac{P_r(E') \Gamma_\alpha^{(12C^J, E')} \Gamma_\gamma^{(12C^J, E')}} {\Gamma(0^+, 1^+)} \quad (16)
\]
where \( E = E_r + E' \) is the three-body kinetic energy and \( \alpha \) is the fine structure constant.

Comparing the methods. In [13], the full three-body method was used to compute the reaction rate for the triple \( \alpha \) process. The \( \alpha-\alpha \) interaction in [17] was used. This leads to the \( ^{12}\text{C} \) spectrum given in [12], which results in good agreement with the experimental data for about 13 different states. In particular, concerning the \( 2^+ \) resonances, the computed \( ^{12}\text{C} \) spectrum includes a low lying one at 1.38 MeV (above the three-body threshold) with a computed width of 0.13 MeV, and a second one at 4.4 MeV with a width of about 1 MeV. Experimentally only a resonance at 3.88 MeV is fully established. In Ref. [12] the resonances are obtained as poles of the S-matrix by use of the complex scaling method [19]. With this method the resonances behave asymptotically as bound states with complex energy, which automatically determines the resonance energy and the corresponding width. The resonance width is then not a parameter but an output of the calculation. The three-body calculation, as described in [13], gives rise to the triple \( \alpha \) reaction rate shown by the thick solid line in Fig. 1. The contributions coming from the \( 0^+ \rightarrow 2^+ \) and \( 2^+ \rightarrow 0^+ \) transitions are shown by the corresponding thin solid lines. The agreement between the total reaction rate and the result given in [9] (open circles in the figure) is reasonably good. For completeness, we show in the figure the contribution from the \( 2^+ \rightarrow 2^+ \) transition (thin dotted curve). This contribution is very small and could actually be neglected.

When the sequential approach is used, and the reaction rate is obtained from Eq. (10), we get the thick dashed curve in the figure. The sequential method described in the present work and in [9] are identical except for the approximation in Eq. (9). The parameters used in the calculations (Table I) are also the same in both cases. The good agreement between the thick dashed curve and the circles in Fig. 1 shows that the approximation in Eq. (9) is accurate. Only a small difference is found for high temperatures since the contribution from the \( 3^+_1 \) resonance in \( ^{12}\text{C} \) is included in [9], but completely neglected in our calculation. Again, the corresponding thin dashed lines show the contributions to the total rate from the \( 0^+ \rightarrow 2^+ \) and \( 2^+ \rightarrow 0^+ \) transitions.

As seen in Fig. 1, the contribution from the \( 0^+ \rightarrow 2^+ \) transition is very similar in the full three-body calculation and the sequential approximation. This is due to the narrow \( 0^+_2 \) Hoyle three-body state in \( ^{12}\text{C} \) which heavily dominates the full calculation. It has a large strength corresponding to strong population and subsequent decay into the bound \( 2^+ \) state plus a photon. This process is precisely as assumed in the sequential description, and in fact the reason for its success.

However, the lowest \( 2^+ \) resonance in \( ^{12}\text{C} \) (both the one obtained in the three-body calculation and the one used
in \cite{9}) is rather wide, which means that the continuum non-resonant three-body \(2^+\) states can contribute significantly to the \(2^+ \rightarrow 0^+_1\) transition. In fact, as seen in the figure, the three-body and the sequential calculation differ for this contribution, especially at low temperatures. Due to this discrepancy the two computed total reaction rates do not fully agree for temperatures from about 2 to 5 GK. When the temperature increases the thin solid and thin dashed curves in Fig.4 become closer and closer, in such a way that for temperatures higher then 5 GK the total reaction rate is similar in both calculations.

\begin{center}
\includegraphics[width=\textwidth]{fig2.png}
\end{center}

**FIG. 2:** Upper part: the \(dB/dE\) function for the \(2^+ \rightarrow 0^+_1\) transition for the sequential approach as given in Eq.(16) (dashed curve) and the three-body calculation (solid curve). Lower part: Integrands of Eq.(5) (thick curves) and Eq.(10) (dashed curve) and the three-body calculation (solid curve).

As seen in the upper part of the figure, the full three-body calculation accumulates part of the strength at smaller energies than the sequential calculation. This is first of all due to the different resonance energies of 1.38 MeV in the three-body and 1.75 MeV in the sequential calculation. For this reason, for low temperatures, i.e. for \(T \leq 3\) GK, where the integrand is vanishingly small for \(E > 2\) MeV (see the solid curves in the lower part of the figure), the three-body calculation provides a higher reaction rate than in the sequential approximation. The integral of the thick solid line in the lower part of Fig.2 is almost twice the one of the thin solid curve. When the temperature increases, the energy at which the integrand begins to vanish also increases, and the sequential reaction rate adds more strength compared to the three-body case. As a consequence both reaction rates approach each other, and they even cross at some point. The integral of the thin dot-dashed curve in the lower part of Fig.2 (sequential case for \(T=9\) GK) is about 25% bigger than the one of the thick dot-dashed curve (three-body case for \(T=9\) GK). Even for \(T = 9\) GK the integrand only allows contribution up to energies around 5 MeV, which means that the behavior of the \(dB/dE\) function for \(E \geq 5\) MeV is rather unimportant.

Thus, from Fig.2 we can conclude that the full three-body calculation shifts part of the strength to large energies, which contribute very little to the reaction rate. For this reason, for the same low lying \(2^+_1\) resonance energy in \(^{12}\text{C}\), the full three-body calculation provides a smaller reaction rate than the sequential calculation. Or, in other words, for the three-body and sequential calculations to provide the same reaction rate, the \(2^+_1\) resonance energy has to be smaller in the three-body case, in order to compensate the non-contributing part of the strength at large energies (for instance 1.38 MeV in the three-body calculation).
The $2^+_2$ resonance energy and the reaction rate. As seen in Fig.1 for temperatures below about 3 GK the reaction rate of the triple $\alpha$ reaction is dominated by the $0^+ \rightarrow 2^+_1$ transition, and the precise energy of the lowest $2^+_2$ resonance in $^{12}$C does not play any role. Only for temperatures beyond 4 GK the energy of the $2^+_2$ resonance has a sizable effect.

The total reaction rate in the sequential case for different energies of the lowest $2^+_2$ resonance in $^{12}$C. The energy increases from the upper curve to the lower one from 1 MeV up to 5 MeV. The dotted curve is the calculation where the contribution from the $2^+ \rightarrow 0^+_1$ transition has been completely removed.

Fig.3 shows the total sequential reaction rate for different energies of the $2^+_2$ resonance in $^{12}$C. The rate decreases progressively when the resonance is placed at a higher and higher energy. This happens because the higher the energy of the $2^+_2$ resonance, the more strength is added at high three-body energies, where the integrand is small due to the exponential in Eq.(5) or (11) (see the lower part of Fig.2). In fact, for a resonance energy of 5 MeV the computed rate is quite similar to the one obtained when the resonance is removed. Only for temperatures beyond around 7 GK some difference appears.

For the same reason, the same behavior is found for the three-body calculation. An increase of the $2^+_2$ resonance energy decreases the reaction rate. However, full removal of the $2^+_2$ resonance in $^{12}$C gives a rate that differs quite a lot from the one obtained when the full contribution from the $2^+ \rightarrow 0^+_1$ transition is removed. This can be seen in Fig.4 where the thick solid line is the same calculation as in Fig.3 (with the $2^+_2$ resonance at 1.38 MeV), the thick dashed line is the calculation after removal of this $2^+_2$ resonance, and the thin solid line is the result when the full $2^+ \rightarrow 0^+_1$ transition is excluded. The difference between the thin solid line and the thick dashed line in the figure shows the importance of including the additional continuum $2^+$ states in $^{12}$C.

It is important to keep in mind that the three-body calculation, together with the $2^+_2$ resonance at 1.38 MeV, includes as well all the other states obtained in [12], in particular the $2^+_3$ resonance around 4 MeV. For this reason, the thick dashed line in Fig.4 where the resonance at 1.38 MeV has been suppressed, still contains the contribution of the one at about 4 MeV, which is the one experimentally known. Then the thick dashed curve in the figure gives a lower limit to the triple $\alpha$ reaction rate, since this is what we would get in case that the $2^+_1$ resonance in $^{12}$C around 1.5-2.5 MeV is shown not to exist.

In this connection it is interesting to compare the thick dashed line in the figure with the thin dashed line, which represents the reaction rate obtained in the sequential approach when the lowest $2^+_2$ resonance in $^{12}$C is placed at 4 MeV. This is very close to the energy of the lowest $2^+_2$ resonance fully confirmed experimentally, and therefore this would be what provided by the sequential calculation in case that the $2^+_1$ resonance in $^{12}$C around 1.5-2.5 MeV does not exist. The difference between both dashed curves shows the effect of the non-resonant $2^+$ states in this case.

For illustration we also show in Fig.4 the reaction rate that we obtain when the Hoyle resonance is removed from the calculation (dotted curve in the figure). As we can see, this state is responsible for an increase of the reaction of about two orders of magnitude for temperatures below 3 GK.

Thus, from Fig.4 we can conclude that in case that the low-lying $2^+_2$ resonance is confirmed not to exist (such that the lowest one is the already known resonance close to 4 MeV above threshold) the sequential approach would underestimate the triple-$\alpha$ reaction rate. The non-resonant $2^+$ states in $^{12}$C are enough to increase significantly the rate at high temperatures.
Summary and conclusions. We investigate the reaction rate for the triple $\alpha$ reaction. We used the full three-body calculation described in [13] and the sequential description of [9]. For the same set of three-body resonances we find that the full three-body calculation gives smaller rates than the sequential approximation for temperatures above $\sim 3$ GK.

We focus on the importance of the experimentally uncertain lowest $2^+_2$ resonance in $^{12}$C which to a large extent determines the reaction rate for temperatures above 3 GK. Different theoretical calculations predict a $2^+_2$ resonance in $^{12}$C at around 1.0-2.5 MeV, respectively, the computed total reaction rates are quite similar for the whole range temperature. The only exception is for temperatures ranging between about 2 and 5 GK, where the full calculation gives a rate slightly above the one obtained with the sequential calculation. The reason for this behavior is that part of the strength in the three-body case is moved to higher energies due to the higher $2^+_2$ resonances and non-resonant continuum $2^+$ states. The high energy part of this strength contributes very little, and the missing low-energy strength has to be compensated by a lower-lying $2^+$ resonance. For the same energy and width of the $2^+_2$ resonance, the full three-body calculation contributes less than the sequential approximation.

If the lowest $2^+_2$ resonance in $^{12}$C by chance should be at about 4 MeV, where the lowest established $2^+$ state is located, then the reaction rate is higher for the full three-body calculation than obtained from the sequential approximation. This is due to contributions from the non-resonant continuum states in the three-body calculation and the insignificant contribution from a high-lying resonance in the sequential calculation. The numerical result can be taken as a lower limit to the reaction rate, which for high temperatures can be up to about one order of magnitude above the result obtained in the sequential picture.

Summarizing, a detailed description of the triple $\alpha$ reaction rate for temperatures beyond 3 GK requires a careful treatment of the $2^+_2 \to 0^+_1$ transition. The non-resonant $2^+_2$ states, not included in the sequential description, are very important. For a given energy of the lowest $2^+_2$ resonance in $^{12}$C below about 3 MeV, a sequential description of the process overestimates the reaction rate. For a larger resonance energy the rate of three-body calculation exceeds that of the sequential approximation due to the contribution of the non-resonant continuum states.

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