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-INTRODUCTION AND REVIEW-

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MUON-CATALYZED FUSION THEORY
-INTRODUCTION AND REVIEW-

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ABSTRACT

Muon-catalyzed fusion (μCF) has proved to be a fruitful subject for basic physics research as well as a source of cold nuclear fusion. Experiments have demonstrated that over 100 fusions per muon can be catalyzed by formation of the dtμ molecule in mixtures of deuterium and tritium. After a brief review of the subject’s history, the dtμ catalysis cycle and the principal relations used in its analysis are described. Some of the important processes in the μCF cycle are then discussed. Finally, the status of current research is appraised.

1. INTRODUCTION

Muon-catalyzed fusion (μCF) entails the synthesis of accelerator and reactor technology with the atomic, molecular, and nuclear physics of the catalysis cycle. This paper will deal with the reactions in the cycle rather than the creation of muons or collection of the energy. Experiments in the last few years have achieved over 100 fusions per muon in deuterium-tritium mixtures at or near liquid densities [1,2]. However, the fascinating history of the subject began much earlier.

In 1947, only ten years after the discovery of the muon and before it was known for sure that the muon and pion were different particles, the possibility of μCF was hypothesized by Frank [3]. It was a great thrill to hear Sir Charles Frank discuss his ingenious theoretical conception of μCF in the preceding talk. Shortly after Frank’s conception of μCF, Sakarov discussed the possibility of energy production with dtμ and later Zeldovich reinvented and amplified the idea. These theoretical speculations were unknown to Alvarez et al [4] when they accidentally discovered and correctly interpreted p d μCF in the Berkeley bubble chamber. Jackson [5] upon reading about Alvarez’s exciting discovery in the New York Times proceeded to make a fairly thorough analysis of energy production possibilities. More detailed experimental and theoretical investigations quickly followed [6], and the next breakthrough was made possible by Vesman’s [7]
inference from some of these experiments of the existence of a resonant mechanism for forming the ddμ molecule. Armed with this mechanism, Gershtein and Ponomarev [6] predicted a rapid formation rate for the dtμ molecule would enable ~ 100 d–t fusions per muon. The rapid molecular–formation rate was confirmed by Bystritsky et al. [9] in 1980. In 1983 Jones et al. [10] measured a large number of fusion neutrons and demonstrated the temperature dependence of d–t μCF. Today we know that the d–t μCF cycle is far more intricate than could have ever been imagined by these early researchers [10].

Muon–catalyzed fusion has actually been observed for all pairs of hydrogen isotopes except two protons. However, ddμ and dtμ are special in having resonantly enhanced molecular–formation rates. Furthermore, d–t μCF is unique in having a small muon loss via "sticking" to the charged fusion particle. Although all the reactions are of fundamental interest, e.g., d–d μCF for its breakdown of the expected "mirror symmetry" relation [11], this paper will mainly discuss d–t μCF.

In the d–t fusion reaction, an α particle and neutron are produced with the release of 17.6 MeV of energy. Normally this reaction occurs only in energetic beams or hot plasmas because of the Coulomb barrier between the two nuclei. However, if it were possible to get the d and t close enough together otherwise, fusion could occur without all this effort. One might think that the ordinary DT molecule ("dtec") could provide a suitable site, but it turns out that the d and t would not be expected to tunnel from their equilibrium distance to a distance of a few fermi, where fusion can occur, in the entire age of the universe! The muon, except for its finite lifetime, is like a heavy electron and can also bind d and t with an internuclear distance about 200 times shorter corresponding to its 207 times greater mass. In the muonic molecular ion dtμ, tunneling is still necessary but occurs in just a picosecond.

The basic catalysis cycle is characterized by two parameters:

\[ \lambda_c = \text{the cycling rate} \tag{1a} \]

and

\[ \omega_a = \text{the fractional loss per cycle}. \tag{1b} \]

In the d–t μCF cycle, production of fusion neutrons occurs at the (average) rate \( \lambda_c \) until cycling is terminated by the muon sticking to the fusion α particle with probability \( \omega_a \) or by muon decay. Section 2 gives an overview of this cycle and the formulas used for its analysis. Some of the important processes involved are discussed in Secs. 3–5. Needs for future work are mentioned in Sec. 6.
2. THE d-t MUON–CATALYZED FUSION CYCLE

Figure 1 shows a schematic diagram of the d-t MCF cycle. The process starts with a free muon, injected into a gas or liquid mixture of deuterium and tritium, being stopped to form a muonic atom. The slowing and capture occurs primarily by ionization, e.g.,

$$
\mu + D \rightarrow \begin{cases} 
\mu + d + e \\
\text{d}\mu(n) + e 
\end{cases}
$$

(of course, the actual targets are molecular), and it is now known that the muon is slowed to an energy of ~ 10 eV and then captured into an orbital with principal quantum number $n \gtrsim 14$ [12]. If the muon is first captured by d, it has to be transferred to t, an irreversible process since the increase in binding energy greatly exceeds the target temperature,

$$
d\mu(n) + t \rightarrow t\mu(n) + d + \frac{48}{n^2} \text{eV}.
$$

Next, in a collision with $D_2$ or DT, the muonic atom becomes a muonic molecule. This process can occur resonantly, i.e., the binding energy of the dt\mu goes into rovibrational
excitation of the electronic molecule, e.g.

\[ t\mu + D_2 \rightarrow [(dt\mu)_{J,v}, dee]_{K,\nu}, \]  

where \( J,v \) and \( K,\nu \) designate the rotational and vibrational quantum numbers of the muonic and electronic molecules, respectively. In the compound molecule \([(dt\mu)\text{dee}]\), the d:mu is so small compared with the electronic molecule that, for most purposes, it can be considered to be a mass-5 isotope of the hydrogen atom. In this reaction the reduced mass and the rovibrational wave function changes, but the electronic wave function is mostly left alone.

The resonant complex is usually stabilized by conversion of an Auger electron. This process takes the dt\mu molecule from the \( J=1 \) state in which it is initially formed to a \( J=0 \) state where fusion ensues [13]. Upon fusion the muon is usually freed to catalyze another cycle but sometimes sticks to the \( \alpha \) particle,

\[
\begin{array}{c}
\downarrow 1-\omega^a_s \\
\downarrow \omega^a_s \\
n + \alpha + \mu \\
n + \alpha \mu
\end{array}
\]

In the latter case, if it is not liberated before the \( \alpha \mu \) slows down, it is lost forever. However, the \( \alpha \mu \) initially has a high velocity (5.83 a.u.), so the cross sections for stripping, e.g.

\[ \alpha\mu + d \rightarrow \begin{cases} \alpha + d\mu \\ \alpha + d + \mu \end{cases}, \]

are significant. The "reactivation" probability is designated \( R \), and the effective sticking introduced in (1b) is given by

\[ \omega^a_s = \omega^a_s (1-R). \]

Of course, the muon can also decay at any point in the cycle. While basically correct, the cycle shown in Fig 1 is a simplification. In actuality, there are side chains involving d-d and t-t fusion as well as a great variety of processes involving excited states, finite thermalization times, etc.
The usual analysis of the d-t $\mu$CF cycle assumes a steady state. With this assumption, we have a simple expression for $Y_n$, the average number of fusions per muon [14],

$$\frac{1}{Y_n} = \frac{\lambda_0}{\lambda_c} + W,$$  \hspace{1cm} (8)

where $\lambda_0 = 0.5 \times 10^6 \text{ s}^{-1}$ is the muon decay rate, $\lambda_c$ is the cycling rate, and $W$ is the fractional loss per cycle. It can be easily seen from this relation that the average number of fusions per muon is limited by the ratio of the cycling rate to the muon decay rate as well as by the inverse of the loss fraction. Interestingly, these two limits are numerically similar, both $\sim 300$ fusions, under the current optimum experimental conditions (tritium fraction $C_t \approx 0.4$, density $\varphi \approx 1$ relative to liquid hydrogen density, and temperature $T \lesssim 300$ K).

The cycling rate $\lambda_c$ is simplified by the fact that the muon atomic capture (2) and fusion (5) times are very short. Hence, most of the cycle time $\tau_c$ is spent either as $d\mu$ waiting for the muon to transfer (3) or as $t\mu$ waiting to form the molecule (4); i.e.,

$$\tau_c \approx \tau_{d\mu} + \tau_{t\mu}.$$  \hspace{1cm} (9)

In terms of rates [15],

$$\frac{1}{\lambda_c} \approx \frac{q_{1s} C_t}{\lambda_{d\mu} C_t} + \frac{1}{\lambda_{d\mu} C_d},$$  \hspace{1cm} (10)

where $C_t$ and $C_d$ are the tritium and deuterium fractions ($C_t + C_d \approx 1$), $\lambda_{d\mu}$ is the ground-state $d$-to-$t$ transfer rate, $q_{1s}$ is the probability of $d\mu$ reaching its ground state, and $\lambda_{d\mu}$ is the molecular-formation rate. The first term is multiplied by $q_{1s}$ since the transfer rates in excited states are very rapid as is the excited-state cascade. The simple appearance of the $q_{1s}$ factor is somewhat deceptive, it has proved to be difficult to determine experimentally.

The loss term $W$ in Eq. (8) is mainly due to the probability $\omega$ of the muon sticking to the alpha particle, though there are corrections that are especially significant at $\varphi << 1$ or for $C_t^* C_d^* << 1$. 
Fig. 2. Energetics of resonant [(dtµ)de] formation in tµ + D₂ collisions. The energy levels in the potential well on the right hand side are for [(dtµ)de], except the one labeled D₂ which is the ground state of D₂. The resonance condition is satisfied when the kinetic energy ε₀ lines up with one of the rovibrational levels of [(dtµ)de].

\[ W = \omega_s + \text{sticking in other fusion channels } (ddµ \& ttµ) + \text{scavenging by impurities (mainly He)}. \]  

(11)

The sticking factor \( \omega_s \) is further decomposed as in Eq. (7), but \( \omega_s \) and R cannot be determined independently by neutron detection alone. Experiments in which the charged particles a and aµ are observed may be able to achieve this separation.

3. MUONIC MOLECULE FORMATION

From a molecular physics point of view, the most interesting basic process in μCF is muonic molecule formation. Until Vesman's [7] theoretical speculation 20 years ago, it was believed that dtµ was formed by the Auger mechanism [16], e.g.

\[ tµ + D₂ \rightarrow [(dtµ)de] + e^- , \]  

(12)
in which the \( dt \mu \) binding energy is carried off by the ejected electron. The problem with this mechanism is that the rate is slower than the muon decay rate, so usually not even one fusion would be catalyzed.

We now know that there exists a resonant mechanism [Eq. (4)] for forming \( dt \mu \) as well as \( dd \mu \), but apparently not for any of the other muonic molecules. The energetics of this process is illustrated in Fig. 2. The potential energy well on the left is that of \( dt \mu \) showing its state with \( J=1, v=1 \), and on the right is that of the electronic molecule showing several of its rovibrational states. If for some collision energy \( E_0 \) the levels align, as shown, the transition can occur resonantly. The energy balance condition is

\[
E_0 - E_{J,v} = E_{K,v}[\text{(dtp)dee}] - E_{K,v}[D_2].
\]

The prerequisite for the resonant process is that a weakly bound state of the muonic molecule exist with binding energy less than \( E_0 \) comparable to the dissociation energy of the target electronic molecule (\( \sim 4.5 \text{ eV} \)). Early calculations were unable to demonstrate this; e.g., in the Born–Oppenheimer (fixed-nucleus) approximation \( dt \mu \) is much too bound, but in the adiabatic approximation it is not bound at all. Variational calculations [17–19] have now shown that the Coulomb binding of the \( J=1, v=1 \) state of \( dt \mu \) is 0.660 eV. (There also exist four lower lying states of \( dt \mu \), but these play no role in the resonant molecular formation process.) The hyperfine splitting [20] diminishes the binding of the lower hyperfine state, having \( t \) and \( \mu \) singlet coupled, by \( \sim 0.036 \text{ eV} \) and the overall shift due to relativistic and other corrections [20–22] further diminishes the binding by \( \sim 0.026 \text{ eV} \). Accurate calculations of the resonant formation rates require that the binding energy be known to within about \( \pm 0.001 \text{ eV} \).

Since some kinetic energy is required to reach the resonances shown in Fig. 2 (\( \nu' > 2 \) or \( \nu'=2, K' > 2 \)), it was expected that the rate would be slow at low temperature and rise dramatically when the temperature was sufficient to reach the resonance. The rates for \( dd \mu \) formation, measured at several different laboratories, exhibit this characteristic behavior [23]. However, there were two surprises in store when the analogous rate for \( dt \mu \) formation was carefully examined experimentally: (i) the rate does not exhibit a striking temperature dependence (Fig. 3a) [1a] and (ii) the rate has a nonlinear dependence on density (Fig. 3b) [1b]. These surprises have been explained in terms of what can be thought of as "below-threshold resonances," i.e. with \( E_0 < 0 \) in Eq. (13). In the simple-minded picture of Fig. 2, such states are completely inaccessible, however, the resonances are actually broadened by the finite lifetime of the complex \( [(dt \mu)_{11}\text{dee}] \) as well as by three-body interactions [24], e.g.
Fig. 3. Experimental formation rates as a function of (a) temperature $T$ at density $0.15 \leq \rho \leq 0.60$ [Ref. 1a] and (b) density $\phi$ at temperature $T < 130$ K [Ref. 1b]. As is conventional, the rates are normalized to liquid-hydrogen density (LHD = 4.25 $\times$ 10$^{22}$ atoms/cm$^2$), and the density is given relative to LHD. $\lambda_{dt\mu-d}$ is for $t\mu + D_2$ collisions; $\lambda_{dt\mu-t}$ is for $t\mu + DT$ collisions. The normalized $\lambda_{dt\mu-t}$ exhibits no density dependence and is quite small at $T < 130$ K (however, see last paragraph in Sec. 3).

\[ t\mu + D_2 + D_2 \rightarrow [(dt\mu)_{11}\text{dee}] K_2 + D_2 \quad (14) \]

This broadening makes accessible the states with $\nu' = 2$, $K' = 1$ or 2, which have strong transition matrix elements and apparently lie just below threshold [25]. Standard line broadening theory has been adapted [26] for treatment of this process. There is also an indirect way the below-threshold transitions can contribute to molecular formation. Configuration mixing induced by the three-body interactions can enable a weak transition just above threshold to borrow intensity from strong transitions below threshold [27].

It has been generally thought that, although molecular formation from hot $t\mu$ atoms produces a rapid transient [28,29], such epithermal contributions are insignificant at steady state [30]. Recent experiments comparing unequilibrated $D_2/T_2$ mixes with equilibrated $D_2/DT/T_2$ mixes call this belief into question. These experiments demonstrate that $t\mu + DT$ collisions contribute to $dt\mu$ formation at liquid temperature even though the resources for this collision occur only at much higher energies. The simplest interpretation is that the $t\mu$ atoms are not thermalized. This occurrence also is an alternative
Fig. 4. Theoretical kinetic energy distributions [from Ref. 32], calculated by Monte Carlo simulation of the time-dependent Boltzmann equation, of $t\mu$ atoms at various times after initially reaching the ground state in a target consisting of 50% tritium at temperature 30 K. The average time for $dt\mu$ formation is $t = 6$ ns, corresponding to an effective temperature of $\approx 100$ K.

explanation to the above-mentioned lack of a strong temperature dependence of the observed molecular-formation rate. This epithermal possibility depends on the competition between the molecular-formation cross sections and the elastic scattering cross sections discussed in the next section.

4. LOW-ENERGY MUONIC ATOM SCATTERING

Though it has only recently become appreciated, elastic scattering, which determines the rate of thermalization of the muonic atoms $d\mu$ and $t\mu$, may be important for the quantitative understanding of the $\mu$CF cycle. One unconfirmed role [31] may be in the calculation of the fraction $q_{1s}$ in Eq. (10), for which there is a serious discrepancy between experiments and theory. Existing theoretical calculations assume that the $d\mu$ atoms are thermalized before the muon is transferred. If this is not the case, the effective transfer cross sections will be smaller and consequently the value of $q_{1s}$ will be larger. Another process particularly sensitive to the collision energy is resonant molecular formation. As shown in Fig. 4, the distribution can be far from Maxwellian at the average time for molecular formation [32]. However, the elastic cross sections for $t\mu$ used here were calculated for collisions with bare nuclei, $d$ or $t$. Though $t\mu$ is indeed very small compared with the electronic atom, it is now known that the effects of target electronic screening and molecular binding can be quite important at low collision energies—this is illustrated in
Relevant inelastic cross sections include those for muon transfer and for hyperfine quenching. The transfer cross section plays a primary role in determining the cycle time, and its excited state contributions go into the determination of \( q_{1s} \) [34]. Several accurate calculations of the ground-state transfer cross section [17b] have been made and are in good agreement with each other and with experiments, but only approximate calculations of the near-resonant excited-state transfer cross sections exist [34b].

The hyperfine state of \( \mu \) is important because the resonant molecular-formation rates can be quite different for the singlet and triplet states owing to their energy splitting [35]. The different molecular-formation rates for the doublet and quartet hyperfine states of \( \alpha \), and the hyperfine transition rate between them have been clearly seen in d-d \( \mu \)CF experiments [36], but analogous effects have so far been elusive in d-t \( \mu \)CF experiments. Theoretically it is expected that hyperfine quenching is essentially all due to muon exchange in the symmetric collision [37],

\[
t_\mu(\uparrow\uparrow) + t \rightarrow t + t_\mu(\uparrow\uparrow) + 0.24 \text{ eV} .
\] (15)

However, there are some experimental indications [38] that quenching also occurs in the asymmetric collision,

\[
t_\mu(\uparrow\uparrow) + d \rightarrow t_\mu(\uparrow\uparrow) + d + 0.24 \text{ eV} ,
\] (16)
which requires a true relativistic interaction, but the cross section for the latter process has not been calculated yet. As in the case of elastic scattering, electron shielding and molecular binding may affect these inelastic cross sections at very low energies.

5. STICKING AND STRIPPING

The most intransigent limitation of the ability of a muon to catalyze many fusions is the probability \( \omega_s \) that the muon sticks to the charged fusion particle to form muonic helium. As written in Eq. (7), two factors are involved here, the initial sticking \( \omega_s^0 \) and the conditional probability \( 1-R \) that the muon is retained by the \( \alpha \) particle through the slowing-down process.

The simplest calculation of \( \omega_s^0 \) uses the sudden approximation with as initial state the adiabatic united-atom wave function of d\( \mu \) and as final state the various atomic orbitals of \( \mu \alpha \) multiplied by a plane wave factor for the n–\( \alpha \) motion; this simple calculation gives \( \omega_s^0 = 1.16\% \) [39]. Elaborate calculations have now been done in a similar manner but

![Diagram](image_url)

Fig. 6. Experimental and theoretical determinations of sticking \( \omega_s \) as a function of density [LAMPF = Ref. 1b, PSI = Ref. 51, KEK = Ref. 52, Old theory = Ref. 39, Present theory = Ref. 45 for \( \omega_s^0 \) and Ref. 40 for \( \omega_s^0 \)]. Curves through the experimental data points are only meant for guidance.
using the united-atom limit of the nonadiabatic $dt \mu$ wave function; these calculations give $\omega_s = 0.89\%$ \cite{40,21}. The sudden approximation seems to be well justified, but there still remain at least two questionable approximations, namely, ignoring the effect of the nuclear strong interaction on the $dt \mu$ wave function and use of a plane wave for motion that is known to be a d-wave. Preliminary tests of the former, using an optical potential \cite{41,21} and using the nuclear R-matrix boundary condition \cite{42,43}, suggest an effect of only $\sim 5\%$, which in fact increases the sticking rather than improving agreement with the experimental value. The plane-wave approximation remains to be tested \cite{44}.

The early calculation of the reactivation factor $R$ using a simplified kinetic description gave 0.24 with negligible density dependence \cite{39}. As shown in Fig. 6, the first experimental measurements \cite{1} of $\omega_s$ gave values considerably smaller in magnitude than the early theory and displayed a substantial density dependence. Because of this discrepancy, we set out to do more thorough calculations of $R$, which presumably is the only source of density dependence in $\omega_s$. This calculation requires complete treatment of the $\alpha \mu$ kinetics and accurate cross sections, especially for stopping, excitation, ionization, and charge transfer. The rates for the lowest three levels are shown in Fig. 7. The

![Graphs showing rates of LHD for n=1, n=2, and n=3 levels](image)

Fig. 7. Some of the rates (at liquid hydrogen density) used to describe the kinetics of slowing-down $n\mu$ [Ref. 45, except Stark mixing rate from Ref. 40]. The curves are energy loss (light-solid curve), stripping (heavy-solid curves), excitation (long-dashed curves), inelastic deexcitation (short-dashed curves), Auger deexcitation (long- and short-dashed curves), radiation (dash-dotted curves), and $\nu 0 \rightarrow \ell 0$ Stark transitions (dotted curves).
resulting value of \( R \) is significantly greater than the earlier value and does show some density dependence, varying from 0.30 at \( \phi = 0.1 \) to 0.36 at \( \phi = 1.2 \) \[45\]. However, as shown in Fig. 6, the corresponding density dependence of \( \omega \) is only \( \sim 10\% \). A subsequent experiment \[2\] found the same density dependence as the newer theory. The final reconciliation is not yet clear, but it is worth noting that the values of the total loss \( W \) from the two different experiments are in much better agreement than are the values of \( \omega \). The discrepancy may be due in part to different analyses of \( q_{1s} \) \[47\].

The experimental determination of \( \omega \) from the neutron signal is rather indirect. Recent measurements of the charged particles \( \alpha \) and \( \alpha \mu \) \[48\] and of the \( \alpha \mu \) x-rays \[49\] have provided valuable new data. Further charged particle information is anticipated from the new PSI–LNPI collaboration.

6. CONCLUSIONS

After a number of surprises, both experimental and theoretical, the essential features of the d–t muon-catalyzed fusion cycle now seem clear, but some important questions remain.

One of these is the factor \( q_{1s} \) for \( d\mu \) reaching its ground state. Better theoretical calculation of \( q_{1s} \) will require more accurate excited state \( d \rightarrow t \) muon transfer cross sections as well as careful studies of muonic atom thermalization and the excited-state cascade. Determination of the nonthermal energy distribution for \( d \), here, as well as for \( t\mu \) needed for molecular-formation calculations, requires accurate elastic scattering cross sections. The calculations of these elastic cross sections should include the effects of target electronic shielding and molecular binding.

We now have a good qualitative understanding of resonant muonic molecule formation. A nonperturbative calculation of the two-body rate is still desirable. A complete theory of high density (three or more body) effects has not yet been achieved. Accurate calculations of relativistic corrections to the \( d\mu \) binding energy, which needs to be known very precisely for resonant molecular-formation calculations, should soon be available. The comparison with experimentally observed molecular-formation rates is complicated by inadequate knowledge of \( q_{1s} \), \( t\mu \) velocity distributions, and hyperfine quenching rates. More hyperfine quenching in asymmetric collisions, \( t\mu \{11\} \rightarrow d + t\mu \{11\} + d \), seems to be indicated experimentally than is expected theoretically.

For the vital muon sticking factor \( \omega_s \), present theory is 30–50% higher than experiments. The uncertainty due to the theoretical estimates of reactivation is believed to be only \( \sim 10\% \), so the theory of initial sticking (\( \omega_0 \)) is suspect. The effect on \( \omega_s \) due to the
nonadiabatic lag in the $d\mu$ wave function has been accurately taken into account, but there still remain other approximations that need to be checked.

Though this paper has mainly been about the basic physics of $\mu$CF, a few words about the possibilities for application are relevant. With the estimated energy cost of $\sim 8$ GeV to produce a muon [50], breakeven would be achieved at $\sim 450$ fusions/muon. This is about three times the current experimental yield, so energy production in a pure fusion $\mu$CF reactor does not appear possible without further refinements. Externally applied fields can affect both the molecular-formation rate and the stripping and might still make such a reactor possible; further research is desirable. An alternative energy option is a hybrid (fusion/fission) $\mu$CF reactor. Such a reactor has been designed that is claimed to be more efficient than the usual breeder reactor, even with the already observed $\mu$CF yield [50]. Another possibility for practical application is use of the $\mu$CF neutrons to breed tritium.

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DISCUSSION

E.C. Frank: If the 8 GeV for muon production is wall-plug energy, a Carnot factor has to be brought into the determination of breakeven. The fusion energy would only be accessible as heat, so we must use a heat engine and will only be able to make 40% of it available as wall-plug energy. Hence the 450 fusions/muon for breakeven catalytic efficiency would need to be multiplied by a factor of 2.5.

Cohen: That is true if the residual heat is regarded as waste. I should also emphasize that the 8 GeV figure for negative muon production is soft. Other authors prefer 5 GeV and some estimates are as low as 2 GeV.

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