**Table 1: Rate constants for fusion of hydrogen isotopes**

| Reaction | $S(E=0)(\mathrm{Mev-b})$ | $A(\mathrm{cm^3\,s^{-1}})$ |
|---|---|---|
| $\mathrm{p+d \rightarrow {}^3He+\gamma}$ | $2.5\times10^{-7}$ | $5.2\times10^{-22}$ |
| $\mathrm{p+t \rightarrow {}^4He+\gamma}$ | $2.6\times10^{-6}$ | $4.8\times10^{-21}$ |
| $\mathrm{d+d \rightarrow {}^3He+n \oplus {}^3H+p}$ | $1.1\times10^{-1}$ | $1.5\times10^{-16}$ |
| $\mathrm{d+t \rightarrow {}^4He+n}$ | $1.1\times10^{1}$ | $1.3\times10^{-14}$ |

**Table 2: CF rates in isotopic hydrogen molecules**

(Entries are $\log_{10}$ of the rate is $\mathrm{s^{-1}}$)

| | $m^*/m_e=1$ | 2 | 5 | 10 |
|---|---|---|---|---|
| p + d | −55.0 | −36.0 | −19.0 | −10.4 |
| p + t | −57.8 | −37.7 | −19.7 | −10.5 |
| d + d | −63.5 | −40.4 | −19.8 | −9.1 |
| d + t | −68.9 | −43.5 | −20.9 | −9.4 |

## References

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where $n, m$ label the electronic states, which we assume to vary on the scale of the Bohr radius. The local wavenumber at small distances is $k(r) \approx (2\mu/r)^{1/2}$. This term is to be compared with the effect of the diagonal potential at short distances, $\approx \Psi_m/r$, giving a correction to adiabaticity of order $(k/\mu)/(1/r) \approx (r/\mu)^{1/2} \ll 1$.

In summary, we have calculated cold fusion rates in isotopic Hydrogen molecules.

We find that the rate for d + d fusion in the free molecule ($\approx 3 \times 10^{-64}\,\mathrm{s}^{-1}$) is some 10 orders of magnitude larger than the most recent previous estimate [11], but that the rate for p + d is faster yet by some 8 orders of magnitude. This latter remains true for rates slower than $\approx 3 \times 10^{-17}\,\mathrm{s}^{-1}$ ($m^* \approx 6m_e$). Hence, if refs. [5,6] are seeing any nuclear process at all, it is more likely the neutron-free p + d reaction rather than d + d. We also find that hypothetical enhancements of the electron mass by factors of 5–10 are required to bring CF rates into the range of values claimed experimentally. However, we know of no plausible mechanism for achieving such enhancements.

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It is interesting to ask by how much the internuclear separation must be decreased in order to reach the fusion rates claimed in [5,6]. Although the precise answer depends upon the details of the internuclear potential, a simple way of quantifying the problem is to endow the electron with a larger mass $m^*$ than it actually has. The equilibrium internuclear separation then scales as $m_e/m^*$, while Eq. (9) above allows the enhancement to be estimated as

$$\log_{10}\left[\Lambda(m^*)/\Lambda(m_e)\right] = 3\log_{10}\left(m^*/m_e\right) - 79(\mu/M_n)^{1/2}[(m_e/m^*)^{1/2} - 1]\ , \qquad (10)$$

where $M_n$ is the nucleon mass and the logarithmic variation with $m^*$ is due to the scaling of $\Psi(\rho)$. More accurate estimates can be had by numerical integration of the Schroedinger equation (5) with the K–W potential [8,9], as shown in Table 2.

Note that a mass enhancement of $m^* \approx 5m_e$ would be required to bring the CF rates into the range claimed by [6] while $m^* \approx 10m_e$ is required by the results of [5]. These should be taken as only a rough guide, however, as Hydrogen in Palladium is dissociated into atoms and ionized to bare nuclei [12].

It is worth remarking on the validity of the Born-Oppenheimer approximation we have used in our calculations. Since there is a large difference between the potential and total energies in the classically forbidden region, one might naively expect a failure of the adiabatic assumption. However, more careful reflection suggests otherwise. Sytematic corrections to the adiabatic approximation are possible by considering the full coupled-channels generalization of Eq. (5) [13]. The largest coupling terms are of order

$$\frac{1}{\mu}\langle n|\frac{\partial}{\partial r}|m\rangle\frac{d\Psi_m(r)}{dr} \approx \frac{k(r)}{\mu}\Psi_m(r)\ , \qquad (11)$$

For smaller values of $r$ we fitted the calculated values of $V - 1/r$ to a seven term Lagrange interpolation formula. Upon numerical evaluation of the integral using the exact $d + d$ eigenvalue and turning point, we find

$$B = e^{-4.13\sqrt{\mu}} \tag{9}$$

The numerical coefficient of 4.13 is to be compared with the estimate of 3.0–3.3 made by Zeldovich and Gershtein [2]; the difference leads to a penetration factor which is 15-21 orders of magnitude smaller.

An accurate evaluation of the CF rates can be obtained by a direct numerical integration of the Schroedinger equation (5) with the K–W potential, as shown in the second column of Table 2. The nuclear radius was taken as $\rho = 2 \times 10^{-4} (\approx 10\,\mathrm{fm})$. The numerical methods of [10] were used, with the wave function being treated explicitly only for $r > 0.005$; the regular s-wave Coulomb function was used to extrapolate this solution to $r = \rho$.

The exact dependence of the barrier factor on reduced mass that we extract from these results is good agreement with the WKB approximation (7), but disagrees with references [2] and [11]. The estimate of the d + d fusion rate made in [11] is too low by about 10 orders of magnitude, because in the calculation of the WKB penetration integrals an unshifted coulomb potential was used at small separations (i.e., our Eq. (6) with $V_0 = 0$). The effective energy with which the nuclei assault the coulomb barrier is therefore lower than it should be, and hence the calculated fusion rate is smaller. We note that the p + d fusion rate is 7.5 orders of magnitude larger than the d + d rate. Although the nuclear rate constant for p + d is some 5.5 orders of magnitude smaller than for d + d, the smaller reduced mass enhances the tunneling probability more than enough to compensate for this.

with the normalization $\int_0^\infty \psi^2\, dr = 1$. The radial wave function $\psi$ then satisfies the Schroedinger equation

$$[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + V(r)]\psi(r) = \epsilon\psi(r) \tag{5}$$

where $\epsilon$ is the eigenvalue for relative motion. Unless otherwise specified, we will hereafter work in atomic units ($e^2 = \hbar = m_e = 1$), so that all energies are measured in Hartrees ($\approx 27.2$ eV) and all distances are measured in Bohr radii ($a \approx 0.53 \times 10^{-8}$ cm).

Simple considerations determine the general features of $V(r)$. If energies are measured relative to the energy of two isolated Hydrogen atoms ($-1$), $V$ vanishes at large $r$. Further, it must have a minimum of the proper depth and separation to support the observed molecular bound states. At small separations, the electronic structure is that of the He atom with an energy of $V_0 = -1.9037$ relative to two isolated hydrogen atoms, so that

$$V(r \to 0) \to \frac{1}{r} + V_0\ . \tag{6}$$

An estimate of the supression of the fusion rate by tunneling is given by the barrier penetration factor obtained from the WKB approximation to Eq. (5):

$$B = e^{-2\int_0^{r_0} k(r)dr} \tag{7}$$

where the local wavenumber is $k(r) = [2\mu(V(r) - \epsilon)]^{1/2}$ and the integral extends to the classical turning point, $r_0$.

To estimate the barrier penetration integral (7), we have taken for the diatomic molecular potential $V(r)$ the current best available numerical calculation in the Born-Oppenheimer approximation done by Kolos and Wolniewicz (K–W) [8,9]. For $1.1 < r < 3$ this potential is well approximated by the Morse potential

$$V(r) = 0.1745[e^{-2.08(r-1.4)} - 2e^{-1.04(r-1.4)}] \tag{8}$$

embedded in Palladium [5] and Titanium metal [6] have prompted us to reconsider previous estimates of the CF rates for free diatomic isotopic hydrogen molecules.

Consider a free diatomic molecule composed of two hydrogen nuclei (which might be different isotopes). In the Born-Oppenheimer approximation the fusion rate $\Lambda$ is proportional to the probability that the nuclei are very close together:

$$\Lambda = A|\Psi(\rho)|^2 \ , \tag{1}$$

where $\Psi$ is the normalized wave function describing their relative motion The inter-nuclear separation $\rho$ is a typical distance where nuclear interactions occur, approximately 10 fm.

The nuclear rate constant $A$ for a given pair of nuclei is related to the low-energy behavior of the corresponding fusion cross section. If the variation of the cross section $\sigma(E)$ with relative energy $E$ is parameterized in terms of the usual S-factor,

$$\sigma(E) = \frac{S(E)}{E} e^{-2\pi\eta}; \quad \eta = \frac{e^2}{(2E\hbar^2/\mu)^{1/2}} \ , \tag{2}$$

with $\mu$ the reduced mass of the two nuclei, then

$$A = \frac{S(E=0)}{\mu c^2} \ \frac{c}{\pi\alpha} \tag{3}$$

with $\alpha = e^2/\hbar c \approx 1/137$. Table 1 shows the nuclear rate constants for four possible interactions between two hydrogen nuclei [7].

We restrict ourselves only to s-wave nuclear motion (for which the fusion rate will be largest), so that the wave function can be written as

$$\Psi(r) = \frac{\psi(r)}{4\pi r} \tag{4}$$

# Cold fusion in isotopic hydrogen molecules

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We have calculated cold fusion rates in diatomic hydrogen molecules involving various isotopes. An accurate Born-Oppenheimer potential was used to calculate the ground state wave functions. We find that the rate for d + d fusion is $3 \times 10^{-64}\,\mathrm{s}^{-1}$, some 10 orders of magnitude faster than a previous estimate. We also find that the rate for p + d fusion is $10^{-55}\,\mathrm{s}^{-1}$, which is larger than d + d due to the enhanced tunneling in the lighter system. Enhancements of the electron mass by factors of 5–10 would be required to bring cold fusion rates into the range of recently claimed observations.

"Cold fusion" (CF) occurs when two nuclei with very small relative energy tunnel through their mutual coulomb barrier to initiate a nuclear reaction. The phenomenon is well-studied in muon catalyzed fusion [1,2,3], where the large mass of the muon relative to an electron results in tightly-bound diatomic muo-molecules of Hydrogen (e.g., d-$\mu$-t) with cold fusion rates of order $10^{12}\ \mathrm{s}^{-1}$. It is also believed to occur as pycno-nuclear reactions in certain astrophysical environments [4]. Recent reports of CF between hydrogen isotopes