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Atomic Effects on the Tritium *ft* Value

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Atomic effects on the tritium ft value including bound-state decay, imperfect wave-function overlap, screening, and electron exchange are considered for each of the species T^+, T, T_2, and T^-. Corrections to the f value are tabulated and can be combined to extract an improved estimate for the axial-vector matrix element in tritium β decay.

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The ft value or comparative half-life of the triton is related to the vector and axial-vector matrix elements and coupling constants by

$$(ft)^{-1}=(G_V^2|M_V|^2+G_A^2|M_A|^2)\times m^5c^4/2\pi^3\hbar^7\ln2. \qquad (1)$$

The phase-space factor, f, defined in detail below, is a function of the energy W_0 available for the decay, and t is the half-life, $t_{1/2}$. With G_V determined from pure vector decays and the ratio G_A/G_V from neutron decay,[1] measurements of W_0 and $t_{1/2}$ fix the value of M_A.

For example, in a recent paper an "experimental" value for M_A of $\sqrt{3}(0.958\pm0.008)$ was deduced from ft (after corrections for radiative, screening, and other small effects).[2] A value $W_0=18\,619\pm11$ eV for atomic tritium was used to evaluate f, while $t_{1/2}=12.330\pm0.013$ yr was taken as a weighted average of half-life measurements on molecular tritium or tritium salts.[3] If the triton half-life depends on the atomic or molecular environment this procedure is invalid. Indeed, an examination of the precision measurements of $t_{1/2}$ listed in Table I that have greatest weight in determining the average value indicates that this may be the case. Extraction of M_A from the ft product requires greater care. This point is reconsidered below.

The main purpose of this investigation was to attempt to understand the variations in Table I that might be attributed to atomic and molecular effects on f and consequently on $t_{1/2}$.[7] These effects are of four types: (1) bound-state decay in which an electron is created directly in a vacancy in the K or higher shells of ^{3}He, (2) excitation and/or ionization of atomic or molecular ^{3}He as a result of the imperfect overlap of initial and final wave functions, (3) screening of the nuclear potential seen by the emitted β particle, (4) and exchange of an atomic or molecular electron with the β particle. For the bare triton, T^+, bound-state decay is the only correction to the f value. The magnitude of each of the four effects has been examined for T (atomic tritium), T_2 or TH, and T^-.

Bound-state decay.—The ratio of bound-state decay to continuum decay for T is 0.0069, while for T^+ it is 0.0103.[8] These corrections are of the order of the radiative corrections to the continuum decay. For T_2 and T^- the probability to create a K electron can be written as[9]

$$P(N_K)/P_\beta=0.0653(2-N_K)Z'^3/W_0^{3/2}, \qquad (2)$$

TABLE I. Precision measurements of the tritium half-life in different chemical environments. All values are in years. The calorimetry result is based on the five determinations listed below it.

$t_{1/2}$	Method	Source	References
12.262 ± 0.004	Helium collection	Low-pressure T_2 gas	4
12.250 ± 0.027	Helium collection	LiT	3,5
12.346 ± 0.002	Calorimetry		6
12.3452 ± 0.0019		Titanium tritide	
12.3479 ± 0.0030		Titanium tritide	
12.3452 ± 0.0084		Titanium tritide	
12.3583 ± 0.0057		High-pressure T_2 gas	
12.194 ± 0.056		High-pressure T_2 gas	

where N_K is the number of initially present molecular or negative-ion electrons that are localized in K orbits about the daughter ^{3}He nucleus ($N_K = 0, 1, 2$). W_0 is in kiloelectronvolts. The probability for a specific value of N_K can be found from the overlap between initial and final wave functions. For T_2 or TH we take as the initial function[10]

$$\psi(T_2) = C[\psi_A(1)\psi_B(2) + \psi_A(2)\psi_B(1)], \tag{3}$$

with

$$\psi_A(1) = \left(\frac{Z^3}{\pi a_0^3}\right)^{1/2} \exp\left(-\frac{Z}{a_0} r_{1A}\right),$$

$$\psi_B(1) = \left(\frac{Z^3}{\pi a_0^3}\right)^{1/2} \exp\left(-\frac{Z}{a_0} r_{1B}\right),$$

$Z = 1.166$, and $C = 0.586$. The equilibrium nuclear separation for this function is 0.76 Å.

Experiments show that 90% or more of the decays of TH or T_2 result in HeH$^+$ and HeT$^+$ molecular ions.[11] An early calculation of bound-state decay for TH assumed the ^{3}He was a free atom or ion.[9] A simple wave function for the $^1\Sigma$ ground state of HeH$^+$ corresponding to a combination of ionic and covalent bonds is[12]

$$\psi(\mathrm{HeH}^+) = 0.65\,496\psi_a(1)\psi_a(2) + 0.29\,284[\psi_a(1)\psi_b(2) + \psi_a(2)\psi_b(1)], \tag{4}$$

where

$$\psi_a(1) = \left(\frac{c^3}{\pi a_0^3}\right)^{1/2} \exp\left(-\frac{c}{a_0} r_{1a}\right),$$

$$\psi_b(1) = \left(\frac{\alpha c}{\pi a_0^3}\right)^{1/2} \exp\left(-\frac{\alpha c}{a_0} r_{1b}\right),$$

with $c = 1.9252$, $\alpha = 0.7567$. This physically appealing wave function gives a dissociation energy (1.97 eV), internuclear separation (0.758 Å), and overlap with the initial molecular function (0.59) all in excellent agreement with calculations using much more elaborate wave functions.[13] Excited molecular states, if they exist, are weakly bound with estimated internuclear separations of 2.4 Å or greater,[14] and would be sparsely populated because of the Franck-Condon principle. According to Eq. (4), there are always one or two electrons localized about the ^{3}He nucleus. If we use the experimental value of 90% for the overlap we can easily compute that the probability for $N_K = 1$ is $0.9 \times 61\%$, while for $N_K = 1$ it is $0.9 \times 39\%$. Equation (2) with $Z' = 1.9252$ yields $P_K/P_\beta = 0.0020$. This value may underestimate the true bound-state decay rate since dissociated final states which constitute 10% of the decay have been neglected. On the other hand, calculations of bound-state decay for T$^+$ and T based on Eq. (2) are overestimates compared to the more reliably calculated values quoted above by as much as 30%. A further overestimate results from adopting the measured rather than the calculated value for the overlap.

The β decay of T$^-$ is interesting in its own right. In addition, the electronic environment of the triton in the ionic crystal LiT is also well approximated by the T$^-$ wave function which for our purposes is[15]

$$\psi(T^-) = A(a^{-ar_1} e^{-br_2} + e^{-ar_2} e^{-br_1})(1 + cr_{12}), \tag{5}$$

with $a = 1.074\,78$, $b = 0.47\,758$, $c = 0.31\,214$, and $A = 0.03\,122$. Final states will correspond to $N_K = 2$, from the overlap of $\psi(T^-)$ with the helium ground state; $N_K = 1$, where one K electron is retained while the second is in an excited state or in the continuum; $N_K = 0$, for which the K shell is vacant. For the He $(1s)^2$ ground state we take the usual product of hydrogenic $1s$ functions with $Z' = 1.688$. This gives a probability of 19% for $N_K = 2$. A closure calculation yields a probability of 68% for $N_K = 1$, leaving a probability of 13% for $N_K = 0$. Corresponding to $N_K = 0$ we take $Z' = 2$ in Eq. (2), while for $N_K = 1$ a variational calculation of the charge seen by the created particle gives $Z' = 1.75$. We find $P_K/P_\beta = 0.0047$.

Imperfect overlap and screening.[17]—Let φ_i describe the initial system, normally in its ground state, with Hamiltonian H_i and eigenvalue E_i. After β decay the system will be described by a set of eigenfunctions $\varphi_{f,n}$ of the Hamiltonian $H_f = H_i + \Delta V$ corresponding to the eigenvalues $E_{f,n}$. E_i and $E_{f,n}$ do not include rest-mass contributions. ΔV is the change in the potential energy term in H_i. For TH decay $\Delta V = e^2/|\vec{r}_1 - \vec{r}_T| + e^2/|\vec{r}_2 - \vec{r}_T| - e^2/|\vec{r}_T - \vec{r}_H|$ while for T$^-$, $\Delta V = e^2/r_1 + e^2/r_2$. The usual definition for the phase-space factor is

$$f = \int_{mc^2}^{W_0} F(Z, W) pW(W_0 - W)^2\, dW. \tag{6}$$

$F(Z, W)$ is the Fermi function, and $W_0 = M_i c^2 - M_f c^2 + E_i - E_{f,n}$, where $M_i - M_f = \Delta M$ is the difference between initial and final *nuclear* masses. The recoil energy (3 eV) and a possible neutrino mass have not been subtracted. The effect of imperfect overlap of final and initial wave functions and the effect of screening may be incorporated simultaneously by replacing the integral in Eq. (6) by[7]

$$f = \int_{mc^2}^{\Delta Mc^2+V} F(Z, W - \bar{V}_n)\left(\frac{(W-\bar{V}_n)^2 - m^2c^4}{W^2 - m^2c^4}\right)^{1/2} \times \left(\frac{W-\bar{V}_n}{W}\right) pW(\Delta Mc^2 + V - W)^2\, dW, \qquad (7)$$

where $V = -\langle \varphi_i | \Delta V | \varphi_i \rangle$ and $\bar{V}_n = -\sum_n c_n^2 \langle \varphi_{f,n} | \times \Delta V | \varphi_{f,n} \rangle$.

The c_n coefficients are those in the expansion $\varphi_i = \sum_n c_n \varphi_{f,n}$. V and $\bar{V}_n$ differ physically because the distribution of final states affects the average energy available for decay and the screening of the emitted particle in different ways. They differ formally because the $\varphi_{f,n}$ are eigenstates of H_f and not of ΔV.

With the wave functions given above and guided by our closure result for the final-state distribution following T^- decay we compute the values for V and $\bar{V}_n$ given in columns 2 and 3 in Table II. Furthermore, it can be shown that the variations in the phase-space factor with V and $\bar{V}_n$ are given approximately by[16]

$$\frac{\delta f}{\delta V}\frac{1}{f} = 0.0184\%\ \text{per eV}, \qquad \frac{\delta f}{\delta \bar{V}_n}\frac{1}{f} = -0.0055\%\ \text{per eV}. \qquad (8)$$

We consider variations in the phase-space factor starting from T^+ decay for which atomic effects vanish. The values listed in columns 2 and 3 translate to the percent changes in f given in columns 5 and 6.

Exchange.—The direct exchange, in which an initially present 1*s* electron is flipped into the continuum and another 1*s* electron created in its place by β decay, is small.[17] However, the interference between the amplitude for the creation of a continuum electron and the amplitude for the direct exchange is not negligible.[18] The fractional change in f is given approximately by $-2[1-(1-E_K/2E_{\max})^2]$, where E_K is the K electron binding energy.

To summarize, the fractional changes in f due to all the effects considered for each of the four species are given in Table II. Inspection of Table II reveals that $t_{1/2}(T^-) < t_{1/2}(T_2)$ in qualitative agreement with measured values in Table I, if LiT is truly an ionic crystal. Lack of quantitative agreement may be indicative of a decrease in electron density around the T^- ion due to the crystal field or to the partial covalent character of the Li-T bond.[19] Table II clearly demonstrates the necessity for making measurements of both W_0 and $t_{1/2}$ in materials where the atomic and molecular corrections to the f value can be made reliably. This cannot be done for titanium tritide since the phase diagram for the titanium-hydrogen system[20] shows that two phases with different atomic concentrations of hydrogen coexist in the temperature range in which measurements were made.[6] Similarly, the solubility of tritium gas under high pressure in the walls of the container makes the electronic environment of the tritium uncertain.

One important consequence of this discussion is the reevaluation of the axial-vector matrix element M_A mentioned above. Exchange contributions to M_A arise from the presence of mesons and deltas in the nucleus. Table II provides the means for combining the best values for $W_0 = \Delta Mc^2 + V$ based on the atomic mass difference with the best value for $t_{1/2}$ for which corrections to the f value are calculable, namely T_2. For example, the nuclear mass difference $mc^2 + 18\,508 \pm 7$ can be deduced from the atomic mass difference 18 573 ± 7 eV.[21] The average end-point energy, $\Delta Mc^2 + V$, for T_2 according to Table II is 18 537 eV, compared to the recommended value 18 619 eV. Equation (8) indicates a decrease

TABLE II. End-point and screening parameters are given in electronvolts in columns 2 and 3. The remaining columns list the shifts in percent of the phase-space factor due to the particular atomic effect indicated, as well as the total shift.

Species	V (eV)	$\bar{V}_n$ (eV)	$\Delta f/f$ (bound state)	$\Delta f/f$ (overlap)	$\Delta f/f$ (screening)	$\Delta f/f$ (exchange)	$\Delta f/f$ total
T^+	0	0	1.03	0	0	0	1.03
T	27	41	0.69	0.50	−0.22	−0.15	0.82
T_2	29	65	0.20	0.53	−0.36	−0.05	0.32
T^-	37	63	0.47	0.68	−0.35	−0.15	0.65

in the f value compared with that based on 18 619. A further net decrease of -0.21% in the ft value for T_2 is predicted based on the remaining corrections for bound state, screening, and exchange in Table II. However, the value $M_A = 0.958$ in Ref. 2, from which we are scaling, already includes a screening correction of approximately -0.22% for atomic tritium. The further net decrease is therefore unnecessary. If the resultant f is combined with $t_{1/2} = 12.262 \pm 0.004$ yr a value of $M_A = \sqrt{3}(0.970 \pm 0.008)$ is found, which may imply a significantly higher probability for finding delta isobars in the triton.

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