

Improved Molecular Final-State Distribution of HeT^+ for the β -Decay Process of T_2

Alejandro Saenz,¹ Svante Jonsell,² and Piotr Froelich²

¹*Max-Planck-Institute for Quantum Optics, Hans-Kopfermann-Straße 1, D-85748 Garching, Germany*

²*Department of Quantum Chemistry, Uppsala University, Box 518, S-75120 Uppsala, Sweden*

(Received 26 April 1999)

An improved theoretical final-state distribution of HeT^+ (and HeH^+) resulting from the β decay of molecular tritium T_2 (HT) is presented to accommodate the needs of increased accuracy in the analysis of ongoing and future tritium neutrino-mass experiments. The previously available theoretical spectrum has been improved in many respects, and adopted approximations have been validated.

PACS numbers: 31.15.-p, 14.60.Pq, 23.40.Bw

Very recently, evidence for oscillation of atmospheric neutrinos has been reported by the Super-Kamiokande Collaboration [1], implying that neutrinos in fact possess a nonzero rest mass. However, the oscillation experiments do not probe the absolute masses of the neutrinos. Instead, only flavor-mixing angles and differences of squares of neutrino mass eigenstates can be obtained. Although these differences are found to be small, this does not automatically imply that the masses themselves are also small. There is no *a priori* reason to assume that the neutrino mass eigenstates follow the mass hierarchy of the charged leptons, and the Super-Kamiokande results are compatible with nearly equal mass eigenstates. Such a scenario with mass eigenstates of the order of 1 eV/ c^2 would be of paramount importance for cosmology.

In this situation, the next most urgent task is the determination of the masses themselves, and the most promising type of experiment in this respect is the tritium neutrino-mass experiment. There the mass of the electron antineutrino is extracted from the shape of the β spectrum of (usually molecular) tritium by purely kinematical arguments. In fact, experiments of this type were recently able to lower the upper bound for the mass of the electron antineutrino to a few eV [2,3].

The analysis of the tritium neutrino-mass experiments requires, however, a very accurate knowledge of the molecular final-state distribution. This distribution describes the probability that a certain amount of the energy released in the β decay of a T_2 molecule remains as excitation energy in the molecular daughter ion $^3\text{HeT}^+$. It is important to realize that even in the case of an ideal experiment the accuracy of the extracted neutrino mass would be limited by the accuracy of the molecular final-state distribution, and this distribution has to be taken from theory. For this reason, more than a decade ago, a very elaborate final-state distribution for T_2 was calculated [4].

The accuracy of that distribution and the validity of certain underlying approximations have, however, been questioned, because the fit of the neutrino mass squared yielded a negative value which indicated that the measured β spectrum cannot be described by the theoretically predicted one. This initiated a reinvestigation of the final-state distribution in T_2 β decay, leading to the new distribution

reported in this Letter. A further motivation for the present work is the recently improved sensitivity of the experimental setups in Mainz and Troitsk, as well as a proposed experiment [5] aiming for even higher sensitivity.

The purpose of this Letter is to present a molecular final-state distribution for the β decay of T_2 , HT, or a mixture thereof that is sufficiently accurate for the present and proposed future tritium neutrino-mass experiments. The final distribution (presented in Table I) is the result of the detailed studies reported in [6–11]. Special emphasis has been put on the validation of all approximations that have been adopted. The spectrum covers the whole energy range explored by the experiments and, as will be discussed below, is given in a form that is directly adapted to the needs of the experimental analysis. The spectrum surpasses in accuracy all previously existing theoretical data.

The molecular final-state distribution given in Table I is valid for the β decay of a free T_2 (or HT) molecule that is not influenced by any surrounding (such as solid-state effects, electric or magnetic fields, etc.). The spectrum has been evaluated within the sudden approximation, since its validity for the present purpose was demonstrated in [9] (where the corrections to it were calculated explicitly). The effect of electronic excitation through the recoil has been shown to be very small [8], and was omitted in the calculation. The same is true for the effect of a coupling of the electronic and nuclear motions (nonadiabatic effects) which were explicitly considered in [10,11].

The molecular final-state distribution comprises a discrete part below the dissociation threshold of HeT^+ and a continuous part above that threshold. The previous final-state distribution [4] was presented in a mixed form of discrete (binned or integrated) and continuous probabilities. In this paper the spectrum is presented in a uniform way that is directly applicable to the analysis of experiments; i.e., it is given as a finite number of discrete transition probabilities. For this purpose the spectrum has been divided into small bins covering an energy range of 0.1 (up to a transition energy of 18 eV), 1.0 (from 18 to 90 eV), 2.0 (from 90 to 140 eV), and 4.0 eV (above 140 eV). For each bin the average excitation energy and the total transition probability were calculated and are given in Table I. Above the last excitation energy considered, i.e., above

TABLE I. Discretized final-state probability distribution $P(E_i)$ for ${}^3\text{HeT}^+$ (${}^3\text{HeH}^+$) following the β decay of a free T_2 (HT) molecule within the sudden approximation. The mean excitation energies E_i for both isotopes are given relative to the rovibronic ground state of ${}^3\text{HeT}^+$ and the recoil energy for ${}^3\text{HeT}^+$. The spectrum extends to 240 eV after which an atomic distribution may be used (see text for details).

$E_i(\text{eV})$	$P(E_i)(\%)$	$E_i(\text{eV})$	$P(E_i)(\%)$	$E_i(\text{eV})$	$P(E_i)(\%)$
0.053(0.049)	0.0069(0.0000)	36.459(36.467)	1.6434(1.5166)	88.498(88.493)	0.0757(0.0806)
0.124(0.147)	0.0046(0.0000)	37.445(37.457)	0.9037(0.9546)	89.495(89.498)	0.0696(0.0715)
0.247(0.247)	0.0233(0.0000)	38.463(38.467)	0.4989(0.5951)	90.967(90.962)	0.1236(0.1276)
0.351(0.347)	0.0553(0.0000)	39.499(39.485)	0.3978(0.4492)	92.983(92.979)	0.1080(0.1102)
0.442(0.447)	0.0457(0.0000)	40.506(40.504)	0.4124(0.4280)	94.982(94.981)	0.0966(0.0973)
0.556(0.547)	0.2033(0.0000)	41.498(41.502)	0.4152(0.3905)	96.982(96.981)	0.0864(0.0867)
0.665(0.647)	0.1649(0.0000)	42.498(42.494)	0.3925(0.3795)	98.981(98.979)	0.0776(0.0779)
0.759(0.747)	0.3877(0.0000)	43.504(43.486)	0.3457(0.3308)	100.981(100.980)	0.0703(0.0707)
0.850(0.876)	0.3808(0.2252)	44.511(44.474)	0.3186(0.3122)	102.983(102.982)	0.0636(0.0638)
0.937(0.955)	0.6809(0.5814)	45.494(45.495)	0.2701(0.2906)	104.984(104.984)	0.0578(0.0580)
1.048(1.087)	1.1214(1.2129)	46.481(46.494)	0.2713(0.2538)	106.985(106.985)	0.0528(0.0529)
1.143(1.162)	1.0112(0.6216)	47.483(47.472)	0.2481(0.2438)	108.986(108.986)	0.0483(0.0484)
1.249(1.260)	2.4406(0.6313)	48.513(48.452)	0.2412(0.2236)	110.986(110.986)	0.0444(0.0445)
1.359(1.344)	3.2337(3.0441)	49.498(49.445)	0.1907(0.2201)	112.987(112.986)	0.0409(0.0410)
1.451(1.452)	4.0864(9.5173)	50.462(50.472)	0.1938(0.1989)	114.987(114.987)	0.0378(0.0378)
1.552(1.585)	6.8745(5.7372)	51.501(51.513)	0.1760(0.1808)	116.987(116.987)	0.0350(0.0350)
1.657(1.663)	6.6279(6.9898)	52.496(52.491)	0.1575(0.1609)	118.988(118.988)	0.0325(0.0324)
1.745(1.739)	5.1412(5.7803)	53.491(53.494)	0.1541(0.1627)	120.988(120.988)	0.0302(0.0302)
1.834(1.847)	6.5561(7.1064)	54.502(54.507)	0.1485(0.1632)	122.988(122.988)	0.0282(0.0281)
1.940(1.942)	5.4588(4.1076)	55.508(55.512)	0.1557(0.1963)	124.989(124.989)	0.0263(0.0262)
2.044(2.044)	3.7231(3.3984)	56.526(56.531)	0.1895(0.2533)	126.989(126.989)	0.0246(0.0245)
2.144(2.150)	2.5473(2.7572)	57.518(57.520)	0.2427(0.3266)	128.989(128.989)	0.0230(0.0229)
2.244(2.270)	1.6959(1.2274)	58.529(58.535)	0.3357(0.3956)	130.989(130.989)	0.0216(0.0215)
2.344(2.346)	1.1369(1.0046)	59.518(59.507)	0.4095(0.4490)	132.990(132.990)	0.0203(0.0202)
2.510(2.509)	1.6947(1.4798)	60.505(60.501)	0.4714(0.4895)	134.990(134.990)	0.0191(0.0190)
2.762(2.756)	1.0094(0.8381)	61.505(61.506)	0.5034(0.5065)	136.990(136.990)	0.0180(0.0179)
3.009(3.009)	0.5732(0.4292)	62.501(62.504)	0.5152(0.5320)	138.990(138.990)	0.0169(0.0168)
3.257(3.257)	0.2806(0.2117)	63.503(63.500)	0.5442(0.5690)	141.962(141.962)	0.0311(0.0309)
3.507(3.506)	0.1316(0.0985)	64.512(64.496)	0.5859(0.6180)	145.964(145.964)	0.0278(0.0277)
3.757(3.756)	0.0623(0.0446)	65.504(65.496)	0.6617(0.7003)	149.965(149.965)	0.0250(0.0249)
4.083(4.082)	0.0420(0.0288)	66.510(66.507)	0.7094(0.6969)	153.966(153.967)	0.0225(0.0225)
4.579(4.579)	0.0080(0.0054)	67.501(67.497)	0.7404(0.6898)	157.967(157.968)	0.0204(0.0203)
5.132(5.076)	0.0015(0.0009)	68.492(68.488)	0.7164(0.6457)	161.969(161.969)	0.0185(0.0185)
5.647(5.658)	0.0000(0.0002)	69.489(69.488)	0.6563(0.5835)	165.970(165.970)	0.0169(0.0169)
18.500(18.773)	0.0000(0.0001)	70.486(70.487)	0.5620(0.5037)	169.971(169.971)	0.0154(0.0154)
19.500(19.680)	0.0000(0.0016)	71.473(71.475)	0.4691(0.4318)	173.972(173.972)	0.0141(0.0142)
20.696(20.645)	0.0012(0.0125)	72.478(72.485)	0.3680(0.3547)	177.973(177.973)	0.0130(0.0130)
21.658(21.615)	0.0113(0.0618)	73.486(73.487)	0.3049(0.3003)	181.973(181.973)	0.0120(0.0120)
22.627(22.590)	0.0656(0.2137)	74.443(74.447)	0.2210(0.2437)	185.974(185.974)	0.0111(0.0111)
23.598(23.568)	0.2567(0.5507)	75.446(75.469)	0.1928(0.2029)	189.975(189.975)	0.0103(0.0103)
24.573(24.549)	0.7149(1.1046)	76.465(76.465)	0.1761(0.1862)	193.976(193.975)	0.0095(0.0095)
25.550(25.532)	1.4804(1.7838)	77.430(77.428)	0.1530(0.1723)	197.976(197.976)	0.0089(0.0089)
26.529(26.517)	2.3583(2.3800)	78.512(78.518)	0.1215(0.1236)	201.977(201.977)	0.0083(0.0083)
27.510(27.503)	2.9715(2.6793)	79.464(79.474)	0.1390(0.1597)	205.977(205.977)	0.0077(0.0077)
28.493(28.491)	3.0307(2.5894)	80.504(80.522)	0.1216(0.1238)	209.978(209.978)	0.0072(0.0072)
29.478(29.480)	2.5527(2.1803)	81.510(81.515)	0.1422(0.1459)	213.979(213.978)	0.0068(0.0067)
30.464(30.471)	1.8080(1.6225)	82.523(82.504)	0.1384(0.1356)	217.979(217.979)	0.0064(0.0063)
31.455(31.470)	1.1070(1.1150)	83.505(83.503)	0.1368(0.1325)	221.979(221.979)	0.0060(0.0059)
32.490(32.507)	0.7377(0.9290)	84.499(84.497)	0.1316(0.1266)	225.980(225.980)	0.0056(0.0056)
33.557(33.539)	1.0637(1.2964)	85.490(85.493)	0.1153(0.1082)	229.980(229.980)	0.0053(0.0053)
34.534(34.519)	1.9095(1.8714)	86.491(86.499)	0.1076(0.1036)	233.981(233.980)	0.0050(0.0050)
35.492(35.490)	2.2178(1.9702)	87.498(87.480)	0.0921(0.0912)	237.981(237.981)	0.0047(0.0047)

240 eV, the energy-dependent (nondiscretized) spectrum $P(E)$ (in percent) can be approximated to a good accuracy by an atomic tail [9], i.e.,

$$P(E) \approx 14.7 \left(\frac{8e^{-(4 \arctan \kappa)/\kappa}}{\sqrt{1 - e^{-4\pi/\kappa}} (1 + \kappa^2)^2} \right)^2 \frac{dE}{eV}, \quad (1)$$

where $\kappa = \sqrt{(E - 45 \text{ eV})/13.606 \text{ eV}}$. This tail may be discretized according to the needs of a specific experiment.

If the experiment is performed with a mixture of T_2 and HT (as is usually the case), an accurate analysis requires taking into account the isotope effect. Thus the final-state distribution for both isotopes has been calculated. In order to allow a simple analysis for an arbitrary ratio of T_2 to HT, the spectra are presented in such a way that the final-state distribution for the mixture is simply obtained by summing the spectra of T_2 and HT weighted with their relative portion in the mixture. This is, however, correct only if both spectra have a common energy scale. We have chosen to relate both spectra to the energy scale of T_2 . Thus the spectra for both isotopes are given relative to the rovibronic ground state of ${}^3\text{HeT}^+$. In addition, the difference in recoil energy for the two isotopes ($E_{\text{rec}}^{T_2} = 1.72 \text{ eV}$ and $E_{\text{rec}}^{\text{HT}} = 2.58 \text{ eV}$ at 18.6 keV leading to $\Delta E_{\text{rec}} = 0.86 \text{ eV}$) has been incorporated into the table so that both spectra are given relative to $E_{\text{rec}}^{T_2}$.

In the following, a comprehensive summary is given that briefly describes the numerical approach used for evaluating the molecular final-state distribution given in Table I. Also the differences with respect to the previous final-state distribution in [4] will be highlighted.

The electronic wave functions and matrix elements needed for calculating the transition probabilities to electronic bound states have been obtained with an extended version of the program written by Kołos *et al.* and used in their calculations summarized in [4]. This code allows a calculation in prolate-spheroidal coordinates with explicitly correlated basis functions. For the electronic continuum the method reported in [6] was used.

A full account of the calculation of the transition probabilities to the electronic ground state of HeT^+ is given in [11]. In the case of both the T_2 and the HeT^+ ground states the data existing in literature for Born-Oppenheimer potential curves (including, in the case of T_2 , adiabatic, radiative, and relativistic corrections), and electronic transition matrix elements (within the sudden approximation) were found to be sufficiently accurate for the present purpose. After [4] was completed, an improved potential curve for T_2 was evaluated which has been employed in the present paper. Thus, the rovibrational wave functions and the transition probabilities between rovibronic states have all been recalculated for the transitions to the electronic ground state of HeT^+ . Besides the new potential curve, the main difference to [4] was the use of the *relativistic* recoil. Restricting the present approach to a *nonrelativistic* recoil gave extremely good agreement with the results in

[4], confirming the correctness of both implementations. A detailed analysis of how the final-state distribution is affected by the relativistic recoil and also by possibly rotationally excited T_2 molecules can be found in [11].

For transitions to electronically excited states of HeT^+ all transition matrix elements have been recalculated. In that calculation we have used the 104 basis functions and the (R -dependent) nonlinear parameters given in [12] for the T_2 ground state. At the equilibrium internuclear distance $R = 1.40a_0$, this basis yields an energy value that lies minimally ($1 \mu\text{hartree}$) above the value obtained with the basis used in [4], but it allowed the use of the 104-term basis set in the whole range of R values considered in this work. In this way smoother transition matrix elements (with respect to R variation) have been obtained, since discontinuous changes in the basis were avoided. More details on the basis set and its accuracy can be found in [9].

For the five lowest-lying electronically bound but excited states of HeT^+ , three different 400-term basis sets were employed to ensure an optimal description of the individual states. In all cases the potential curves were of higher accuracy than, or at least the same as, the ones used in [4], leading also to improved transition matrix elements. In the case of the four excited states carrying most of the population after β decay of tritium, the full rovibronic wave functions (within the Born-Oppenheimer approximation) have been calculated and used in the evaluation of the final-state distribution. Details of the calculation are reported in [11].

For the higher-lying electronically bound states (including the Rydberg states), as well as for the description of the electronic continuum, we adopted for consistency one common 400-term basis set in the calculation of the final results. However, a second basis set of the same size as well as two smaller basis sets (200 terms) have been used for analyzing the convergence and reliability of the final result. (Details on the basis set and the calculation are given in [9].) The transition probability into the electronic continuum has been calculated by applying a novel implementation of the complex-scaling method [6] that allows for a correct description of the continuum, while in Ref. [4] a simple discretization was used. A correct description of the electronic continuum is of particular importance in the present context, since the spectrum is strongly affected by autoionizing resonances to which roughly two-thirds of the total probability in the electronic continuum is attributed. The resonances (i.e., their positions and widths) have recently been recalculated by means of the R -matrix method [13]. Comparing those results with the ones obtained with the basis set used in this paper, a very good agreement is found for the important resonances. However, in the present calculation only a finite number of resonances are explicitly contained, while the remaining infinite series are approximated by a finite number of pseudostates. The resulting small inaccuracy should be negligible for the present purpose, as has been discussed in [11] for the similar case of the Rydberg states.

While the transitions to the lowest-lying electronic bound states have been calculated in a fully rovibrationally resolved way, such a calculation would be prohibitively difficult for the electronic continuum. Therefore the reflection approximation was introduced for this problem in [9] (where also a detailed derivation and validation is given), which allowed taking into account the effect of the broadening of the spectrum due to nuclear motion. The final calculation is based on 55 spectra calculated at values of the internuclear distance ranging from 0.6 to 4.0 a.u. This is in contrast to [4], where the effect of nuclear motion on Rydberg states and the (discretized) continuum had been taken into account by the cruder approximation of a mean excitation energy, yielding a nonbroadened discretized spectrum. It is possible to demonstrate that the effect of recoil-induced rovibrational excitations can, to a good approximation, be incorporated into the spectrum for all but the electronic ground state via an effective energy shift [9,14]. This shift has been determined to be 1.89 eV for T_2 and 1.14 eV for HT by a comparison of the results obtained for the electronically bound states of HeT^+ , once by the full treatment and once by applying the reflection approximation. (The value of the shift differs slightly from the one in [9], since the improved results for the electronic bound states of HeT^+ [11] were used in the present work.) This shift was completely neglected in [4].

Finally, it is possible to show that the *ab initio* high-energy final-state distribution matches an atomic-type spectrum that is free of any adjustable parameters [9]. This not only confirms the numerical correctness of the present calculation, but allows one to extend the calculated spectrum to any desired excitation energy.

Since the corrections to the sudden approximation were shown to be negligible [9], the final-state spectrum can directly be interpreted in terms of population probability and thus should exactly sum up to 100% (for the case of beyond-sudden approximation treatments, see Ref. [8]). However, adding up all probabilities (including the atomic tail) obtained in the calculation yields 99.83% for T_2 and 99.84% for HT. Considering the fact that this result is obtained after integration over a spectrum that covers the whole energy range from zero to infinity this is an extremely good result (indicating an *absolute* accuracy of about 0.2%).

Nevertheless, a number of tests have been performed in order to investigate the origin of the missing probability. While these tests allowed us to exclude possible sources such as, e.g., the use of different levels of approximation (fully rovibrationally resolved treatment and separately optimized basis sets for five states vs the use of the reflection approximation and a single basis set for the remaining states including the electronic continuum), they revealed that the loss of the 0.17% probability is rather uniformly distributed over the electronic excitation spectrum above the ionization threshold. Thus, the spectrum has been renormalized by lifting only the contribution arising from

the electronic continuum. Because of the broadening by nuclear motion, it is, however, impossible to separate the electronic continuum from the bound part. Thus, in order to make the renormalization transparent (and reversible), the whole spectrum above 40 eV was multiplied by the factors 1.0106 (T_2) and 1.0097 (HT).

Only a complete analysis based on experimental data can reveal the impact of the improved final-state distribution presented in this paper. This is due to the fact that the spectrum is used in a fit procedure and thus its importance depends critically on the experimental parameters and (statistical) errors, as well as on the fit procedure itself. In order to obtain some estimate of the difference expected from the analysis of an ongoing experiment with either the new final-state distribution or the one given in [4], the following simulation was made. Using the typical parameters of the Mainz neutrino-mass experiment, a large number of synthetic experimental spectra (containing artificial statistical errors produced with the aid of a random-number generator) have been produced based on the present final-state distribution for T_2 and assuming a zero neutrino mass. Then the neutrino mass square m_ν^2 was extracted using the previous final-state distribution [4]. Depending on the energy range of the spectrum included in the fit the fitted value of m_ν^2 can be as large as $1 \text{ eV}^2/c^4$. Although this value is below the sensitivity of the present experiments ($\approx 4.5 \text{ eV}/c^2$ for m_ν [2]), it is of the same order of magnitude as the sensitivity of proposed future experiments which are designed to probe the cosmologically interesting neutrino-mass range.

We thank the Mainz neutrino group for many helpful discussions. We also extend special thanks to Ch. Weinheimer for performing the numerical fit simulations. Financial support from the Swedish Natural Science Research Council (NFR) is gratefully acknowledged.

-
- [1] Y. Fukuda *et al.*, Phys. Rev. Lett. **81**, 1562 (1998).
 - [2] H. Barth *et al.*, Prog. Part. Nucl. Phys. **40**, 353 (1998).
 - [3] V.M. Lobashev, Prog. Part. Nucl. Phys. **40**, 337 (1998).
 - [4] O. Fackler, B. Jeziorski, W. Kołos, H.J. Monkhorst, and K. Szalewicz, Phys. Rev. Lett. **55**, 1388 (1985).
 - [5] J. Bonn *et al.*, Nucl. Instrum. Methods Phys. Res., Sect. A **421**, 256 (1999).
 - [6] P. Froelich *et al.*, Phys. Rev. Lett. **71**, 2871 (1993).
 - [7] P. Froelich and A. Saenz, Phys. Rev. Lett. **77**, 4724 (1996).
 - [8] A. Saenz and P. Froelich, Phys. Rev. C **56**, 2132 (1997).
 - [9] A. Saenz and P. Froelich, Phys. Rev. C **56**, 2162 (1997).
 - [10] S. Jonsell, A. Saenz, and P. Froelich, Pol. J. Chem. **72**, 1323 (1998).
 - [11] S. Jonsell, A. Saenz, and P. Froelich, Phys. Rev. C **60**, 034601 (1999).
 - [12] W. Kołos and L. Wolniewicz, J. Chem. Phys. **43**, 2429 (1965).
 - [13] J. Tennyson, J. Phys. B **31**, L177 (1998).
 - [14] S. Jonsell and H.J. Monkhorst, Phys. Rev. Lett. **76**, 4476 (1996).