Accurate Theoretical β-Decay Energy Spectrum of the Tritium Molecule and Its Neutrino Mass Dependence

O. Fackler,[1,2] B. Jeziorski,[3,4] W. Kołos,[3,5] H. J. Monkhorst,[5] and K. Szalewicz[3,5]

[1]*Department of Physics, Rockefeller University, New York, New York 10021*

[2]*Lawrence Livermore National Laboratory, University of California, Livermore, California 94550*

[3]*Quantum Chemistry Laboratory, Department of Chemistry, University of Warsaw, 02093 Warsaw, Poland*

[4]*Department of Applied Mathematics, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada*

[5]*Quantum Theory Project, Departments of Chemistry and Physics, University of Florida, Gainesville, Florida 32611*

(Received 17 June 1985)

The β-decay energy spectrum which results from the decay of one of the nuclei in the T_2 molecule has been computed. An accurate, explicitly correlated basis set was used to describe electronic states of both the parent and the daughter molecules, and effects of nuclear motion have been taken into account. All the channels which meaningfully affect the spectrum have been incorporated, including resonance and scattering channels. The spectra are presented for several neutrino masses. It is shown that the molecular effects are crucial for accurately determining the neutrino mass from a tritium β-decay experiment.

PACS numbers: 31.20.Di, 14.60.Gh, 23.40.-s

The determination of the neutrino mass (or masses) is of considerable importance for physics, astrophysics, and cosmology.[1-3] The (electron anti) neutrino mass can be deduced from a precise measurement of the tritium nucleus β-decay energy spectrum.[4-7] In most such experiments the tritium nucleus is embedded in a molecular surrounding. As first indicated by Bergkvist,[4] and subsequently by many others,[3,5,6,8-11] effects of these surroundings are of primary importance for determining the neutrino mass from the measured data. The T_2 molecule provides one of the best sources for such a measurement.[3,12,13] At least two experiments are presently under way which employ this source.[12,13]

The molecular effects acompanying the tritium β decay have been studied by us in a series of papers.[14-16] In Refs. 14 and 15 we have presented, for various internuclear distances R, accurate electronic spectra of the daughter molecular ion HeT^+ and the transition probabilities from the ground state of the parent T_2 molecule following its β decay. Knowledge of these data is critical for interpretation of the experimental spectrum and for neutrino mass determination. We have shown that the probability of decay into the ground electronic state is 57.4%, into the electronically excited bound states it amounts to 27.8%, and the states in the ionization continuum contribute the remaining 14.8%. The cited numbers have been averaged over the T_2 ground-state vibrational wave function. In Ref. 16 we performed an analysis of the effect of nuclear motion in $^3HeT^+$ on the probability distribution for the electronic states 1–4 and 6. We have included bound rovibrational levels, rotationally predissociative resonances, and scattering states. This precise knowledge of the system is necessary since at least one of the current neutrino experiments is aimed at a resolution of approximately 1 eV.[12]

In the present paper we use the results of our previous work to construct a theoretical β-decay spectrum of the T_2 molecule, covering all the relevant energy range and for various neutrino masses. These numbers can be used in the present and future experiments, and also could shed some light on the interpretation of the well-known experiment of Lubimov and co-workers.[5,17] Our spectrum surpasses in accuracy all the previously available theoretical data.[3,4,9,11,18,19] A more detailed account of the accuracy of the theoretical spectrum will be published later.[20]

The β spectrum of a molecule is usually presented in the form of the Kurie plot.[21] We have generated such plots by use of the formula

$$K(\epsilon;m_\nu)=[\textstyle\sum_n P_n K^2(\epsilon;E_n,m_\nu)]^{1/2}, \quad (1)$$

where $-\epsilon$ is the energy (in electronvolts) measured relative to the end point of the spectrum, m_ν is the neutrino mass (in energy units), E_n is the energy level, and P_n is the probability of transition to this level. The energy E_n is measured with respect to the lowest energy value in a given treatment of nuclear motion. If the electronic spectrum of the daughter ion is used, this lowest energy value is its ground-state energy for the T_2 equilibrium nuclear distance, $E_1(R=1.4$ bohr), or its ground-state energy averaged over the ground vibration of T_2; if the nuclear-motion–resolved data are employed, E_n is relative to the ground rivibronic level of $^3HeT^+$. $K(\epsilon;E_n,m_\nu)$ is a single branch of the plot defined as

$$K(\epsilon;E_n,m_\nu)=(m_\nu+\epsilon-E_n)^{1/2} \times[(m_\nu+\epsilon-E_n)^2-m_\nu^2]^{1/4}, \quad (2)$$

for $\epsilon \geq E_n$, and $K(\epsilon;E_n,m_\nu)=0$ for $\epsilon < E_n$. For the continuous part of the spectrum, the summation in Eq. (1) should be changed to an integration. We have used simply the midpoint rule to perform the integration. This leads to the same summation as in Eq. (1) with $P_n \rightarrow P(E)\Delta E$, where $P(E)$ is the probability density and ΔE is the integration step.

To produce the Kurie plot for different neutrino

masses, it is sufficient to know all the probabilities P_n and the energies E_n. In Fig. 1 we compare Kurie plots obtained for the pure nuclear, atomic, and molecular (T_2) tritium decay processes for an assumed[2,3,5,17] neutrino mass of 30 eV. The molecular plots are presented in three versions: (i) constructed for a fixed value of the internuclear distance ($R = 1.4$ bohr); (ii) obtained from the data for various R averaged over the ground-state vibration of the T_2 molecule; and (iii) same as (ii) except for a complete treatment of the nuclear motion for the most significantly contributing $^3HeT^+$ electronic states, 1–4 and 6. The plot (iii) represents our final results. The function $P_n = P(E_n)$ which leads to this plot is given in Table I. It can be used to construct Kurie plots needed for interpretation of experimental data.

Before discussing the plots presented in Fig. 1, let us describe the data which were used to construct them. The probability distributions connected with the electronic states 1–4 and 6 of the daughter molecular ion, which include a complete account of the nuclear motion, have been taken directly from Tables III and V of Ref. 16. For the remaining states we have performed calculations for $R = 1.0(0.1)2.0$ bohr, using the electronic wave functions of the same type as described in Refs. 14 and 15. This small range of R is sufficient because of the rapid decay of the T_2 ground vibrational wave function. For T_2 the expansion of the electronic wave function was identical to that used in Ref. 14. For HeT^+ a 200-term expansion has been employed. In Ref. 15 it has been shown that the energies of the HeT^+ resonance states can be computed by the stabilization method.[22] These calculations have been extended and, by a better optimization of the nonlinear parameters in the wave function, improved stabilities of the resonance energies have been achieved. Stability of the lowest two resonance states was used as the main criterion in the optimization, with only a small compromise to get reasonable results for a few higher resonance states as well. Full optimizations of the exponents have been performed at $R = 1.0$, 1.4, and 2.0 bohr. For intermediate distances the exponents have been interpolated. The first 100 eigenvalues for HeT^+ are taken into consideration. These eigenvalues span the first 165.7 eV of the spectrum and account for 0.996 67 of probability at $R = 1.4$ bohr. The remaining amount of 0.003 33 is rather uniformly spread over the next 594 eV, with 0.001 38 in the range 165.7–200 eV. The 200-term function discussed above gives slightly different total transition probabilities to the ground, excited, and continuum states (57.4%, 28.4%, and 14.2%, respectively) from these obtained in Ref. 14.

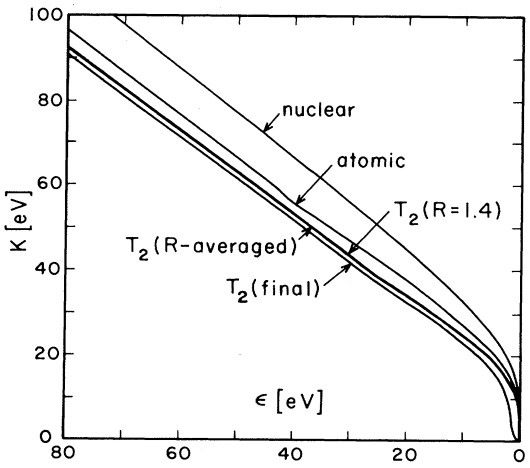

FIG. 1. Comparison of pure nuclear, atomic, and molecular (T_2) Kurie plots for tritium β decay and for $m_\nu = 30$ eV. The curve labeled $T_2(R = 1.4)$ is the one designated as "plot (i)" in the text; $T_2(R$-averaged), "plot (ii)"; and T_2(final), "plot (iii)."

The plot (ii) in Fig. 1 and the contribution from the states 5 and 7-100 in plot (iii) were calculated from the probabilities averaged in the simplest possible way, i.e., the nth root of the Hamiltonian matrix and the probability connected with it were independently averaged over R with the ground vibrational wave function of T_2. The averaged P_n probability was assumed to correspond to the averaged E_n measured with respect to the averaged E_1. For resonance states, one may criticize such an approach since the root number connected with a given resonance state may change with R. This was not the case, however, for the most important, low-lying resonances in our calculations. The small difference at higher ϵ values between the plots (i) and (ii) in Fig. 1 indicates that possible inaccuracies are extremely small.

Figure 1 clearly shows that within the last 3 eV from the end point the molecular effects are much more important than the atomic ones. Because of the spread of the final rovibrational levels in the ground electronic state, close to the end point the final theoretical Kurie plot is practically tangent to the energy axis. This behavior is to be compared with the pure nuclear or atomic decay where the plot is perpendicular to the energy axis. Such a phenomenon does not appear in a molecular calculation which neglects the nuclear motion in the daughter molecular ion [plots (i) and (ii)]. The conclusion is that if the spectrum can be measured sufficiently close to the end point, the atomic effects will become unimportant since they practically do not change the shape of the curve obtained for a bare T nucleus. The nuclear motion effect, however, must be considered in all regions of the spectrum.

In Fig. 2 we present Kurie plots obtained with the probability distribution given in Table I, and for neutrino masses $m_\nu = 0(10)50$ eV. It is seen that the plot becomes practically linear above 100 eV, and is very close to linear already for $\epsilon > 75$ eV, i.e., after inclusion of the contribution from the two main reso-

TABLE I. Probabilities (in percent) for β decay of the T_2 molecule. Energies are given in electronvolts. For energies from 0 to 4.897 eV we give the integral probability P_n for the energy bin from E_n to E_{n+1}. For entries denoted by stars we present the probability density (per electronvolts). For all the other energies, P means the total probability connected with a given energy level.

E	P	E	P	E	P	E	P
0.000	0.008	26.881	2.671*	78.427	0.020	115.612	0.002
0.097	0.005	27.881	3.093*	80.865	0.238	116.455	0.001
0.197	0.028	28.881	2.913*	81.965	0.137	117.594	0.005
0.297	0.055	29.881	2.276*	83.170	0.212	118.481	0.023
0.397	0.056	30.881	1.503*	83.429	0.151	119.245	0.023
0.497	0.218	31.881	0.882*	84.218	0.112	120.360	0.009
0.597	0.191	32.881	0.727*	86.123	0.014	121.764	0.013
0.697	0.434	33.881	1.389*	87.374	0.010	123.594	0.009
0.797	0.429	34.881	2.175*	88.259	0.009	124.247	0.005
0.897	0.688	35.881	2.086*	88.876	0.013	125.709	0.012
0.997	1.300	36.881	1.310*	89.871	0.026	127.715	0.003
1.097	1.078	37.881	0.676*	90.690	0.023	129.373	0.002
1.197	2.793	38.725	0.010	91.784	0.052	130.271	0.004
1.297	3.715	38.881	0.416*	93.247	0.178	132.887	0.060
1.397	4.480	39.881	0.370*	94.333	0.133	133.402	0.025
1.497	7.176	40.881	0.350*	96.192	0.026	134.813	0.082
1.597	6.825	41.881	0.269*	96.701	0.054	135.371	0.006
1.697	5.171	42.732	0.965	97.543	0.023	136.379	0.005
1.797	6.187	42.881	0.166*	98.514	0.005	136.916	0.003
1.897	5.023	43.405	0.029	98.840	0.010	138.243	0.008
1.997	3.334	43.881	0.091*	100.263	0.014	139.737	0.010
2.097	2.239	43.963	0.372	100.784	0.003	141.093	0.006
2.197	1.483	44.147	0.128	101.620	0.003	142.461	0.047
2.297	1.008	44.881	0.043*	102.426	0.005	144.001	0.004
2.397	1.562	45.881	0.016*	102.842	0.001	144.391	0.007
2.647	0.940	46.881	0.004*	103.170	0.001	147.073	0.021
2.897	0.518	47.913	0.129	103.594	0.006	148.311	0.015
3.147	0.249	50.599	1.216	104.236	0.002	148.895	0.001
3.397	0.116	52.553	0.440	105.008	0.001	150.849	0.004
3.647	0.055	55.109	0.065	105.799	0.002	151.442	0.001
3.897	0.036	55.852	0.154	106.990	0.006	152.854	0.000
4.397	0.007	57.004	0.159	108.711	0.010	154.169	0.002
4.897	0.001	62.092	2.634	109.189	0.008	156.093	0.001
20.881	0.003*	67.886	6.029	109.975	0.007	157.003	0.003
21.881	0.021*	71.725	0.306	111.148	0.005	158.134	0.003
22.881	0.109*	74.820	0.245	112.339	0.013	159.271	0.002
23.881	0.385*	75.169	0.088	113.145	0.010	162.054	0.007
24.881	0.973*	75.868	0.100	113.882	0.005	164.173	0.002
25.881	1.833*	76.221	0.273	114.892	0.002	Sum	99.489

nance states (see also Table I). The nuclear motion effects are significant for all the masses considered.

Strictly speaking, the results presented above refer to gaseous T_2 only. One can show,[23] however, that in the case of frozen T_2, as used in the experiment of Ref. 12, the fractional change of the T_2 wave function, $\Delta\psi/\psi$, caused by the binding in the crystal lattice, amounts to less than 0.1%. Some solid-state effect can be anticipated for the final states of the HeT^+ ion due to interactions with the dipole induced by this ion. However, since the distances between molecules in solid T_2 are large and the polarizability of T_2 is small, these interactions will shift HeT^+ energy levels by less than 1 eV. Since the shift should be similar for the most important states, the net effect will be much smaller than 1 eV. This last argument follows from the fact that if the shift had been identical for all the levels, it would have had no effect on the neutrino mass. Hence our results should apply to the condensed T_2, at least for experiments with accuracy not better than about 1 eV.

There are several physical and numerical approximations in the theoretical probability distributions which lead to the Kurie plots. We were able to reduce most of the errors to an insignificant level. An even higher than necessary accuracy of the electronic bound states has been demonstrated in Ref. 14. The adiabatic approximation, which we used for separation of the electronic and nuclear motion, is known[24] to give results for the considered systems which differ negligibly from those obtained in the complete nonadiabatic treatment. The equations for the nuclear motion have

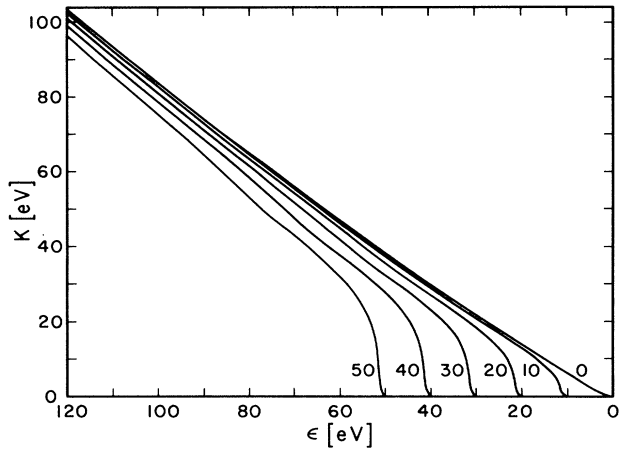

FIG. 2. T_2 β-decay Kurie plots for various neutrino masses. To visualize the differences better, each plot is shifted by m_ν. For large ϵ, $K(\epsilon;m_\nu) \simeq \epsilon - 19.5$.

been solved accurately enough to introduce no additional error; this was checked by employment of various sum rules.[16] Since the electronic states 1–4 and 6, for which the nuclear motion in $^3HeT^+$ has been considered, give 84.2% of the probability, and affect the most important part of the β spectrum, it is entirely sufficient for the remaining states to account for the nuclear motion in the average way.

The accuracy of the transition probability above the ionization threshold is lower. There is some unavoidable arbitrariness in the positions of the resonance states and the scattering states are not well described at all. Fortunately, the probability connected with the latter states is only about 5% and it is quite uniformly distributed. In fact, we have found that reasonable changes of both the energies and transition probabilities for all the states in the continuum (caused, e.g., by variations of the exponents) have practically no effect on our final result.

The main source of error in our theoretical Kurie plots seems to arise from the neglect of the interaction between the β electron and the molecular electrons in the Fermi "golden-rule"-type formula [Eq. (2) of Ref. 16] on which the calculations were based. Using Williams and Koonin's[25] results we have argued[16] that this may lead to an error in the probability amounting to only about 0.2%.

We conclude, therefore, that the accuracy of the results presented in this paper is sufficient for interpretation of the experiments presently under way and for those which may be carried out in the foreseeable future.

This work was performed under the auspices of the U. S. Department of Energy by Lawrence Livermore National Laboratory under Contract No. W-7405-ENG. It was also supported in part by grants from the Division of Sponsored Research of the University of Florida, National Science Foundation Grant No. CHE-8207220, and Polish Academy of Sciences Grant No. MR.I.9. We also thank the Particle Physics Group at the Rockefeller University for providing access to their computational facilities.

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