Widths of the 6.92 and 7.12 MeV levels in ^{16}O and the influence of the effective temperature

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(Received 22 October 1984)

The radiative widths of two ^{16}O levels were determined using photon scattering and self-absorption measurements. The results were $\Gamma_0(6.917) = 0.094 \pm 0.004$ eV and $\Gamma_0(7.117) = 0.054 \pm 0.004$ eV. The effective temperature T_e of the O atom in a water target is calculated by accounting for the effect of the zero-point molecular vibrations of the O atom. The influence of this new value of T_e on the Doppler broadening of the nuclear level and hence on the resulting value of Γ_0 as deduced from a self-absorption measurement is discussed.

The radiative widths of the 6.92 MeV (2^+) and the 7.12 MeV (1^-) levels of ^{16}O are of great interest both theoretically and experimentally. The ^{16}O is a double magic nucleus and several theoretical calculations were carried out to reproduce the measured widths.[1-3] Large discrepancies of $\sim 20\%$ exist in the literature between the several reported measured widths of those levels. Two techniques were used in such measurements: inelastic electron scattering and nuclear resonance fluorescence (NRF). In an attempt to resolve the discrepancies, we remeasured the above widths using the NRF technique trying to avoid possible pitfalls in the process of analyzing the data. In addition, we used, where possible, a self-absorption measurement which is known to yield a more accurate result than that obtained by an absolute scattering cross section measurement. This is because in self-absorption there is no need to know the absolute intensity of the incident photons which usually contributes the largest uncertainty in measuring Γ_0, the ground state radiative width. The determination of Γ_0 by self-absorption requires, however, an accurate value of the effective temperature T_e of the scattering atom. The quantity T_e appears in the expression of the Doppler width $\Delta = E(2kT_e/Mc^2)^{1/2}$ where E is the excitation energy of the nuclear level, and M is the nuclear mass. It was noted in previous publications[4,5] that the normal procedure of calculating T_e by using the Lamb formula[6,7] is not applicable to the present case. This is because the T_e given by Lamb is correct mainly for the case of metallic targets where the Debye approximation of continuous frequency distribution applies. In the case of ^{16}O, the target can occur only in a molecular form, such as O_2 and H_2O, where one should account for the contribution of discrete frequencies to the Doppler width of the ^{16}O nuclear level and hence on its value of T_e. The discrete frequencies correspond to the normal modes of vibrations of the molecule and contributes to T_e through the *zero-point* kinetic energies of the vibrational modes.

The calculation of T_e for such cases was treated by Moreh, Shahal, and Volterra[4] and it was found that the above effect gives rise to a much larger value of T_e and hence to a much higher deduced value of Γ_0 than would be obtained by following the normal procedure.[6,7] If we take as a concrete example a water target, it turns out that by accounting for the vibrational kinetic energy of ^{16}O (including that of its zero-point vibrational motion) occurring in the

H_2O molecule, one obtains $T_e \simeq 410$ K at room temperature (see below) instead of $T_e = 300$ K as usually assumed.[8] The use of the larger value of T_e in a self-absorption measurement leads to larger values of Γ_0 by a factor $(\frac{410}{300})^{1/2} = 1.17$. The calculation of T_e of ^{16}O in water is explained below.

To calculate T_e, which is related to the instantaneous kinetic energy[4] of ^{16}O in H_2O, one should distinguish between the "internal" kinetic energy of ^{16}O due to the normal modes of vibrations of the H_2O molecule and the "external" kinetic energy due to the motion of the H_2O as a whole with respect to the other surrounding molecules. The procedure for calculating T_e for a target in a molecular form was described elsewhere.[4] Here, there are additional difficulties because the problem of the structure and the dynamics of water molecules is complicated by the effect of the hydrogen bonds.[9] Further, since the levels have short lifetimes, things can be greatly simplified if we restrict ourselves to the ^{16}O motion on a time scale of $10^{-14}-10^{-15}$ s. On such a time scale, the water molecules exhibit properties similar to those of a solid[9] having a Debye temperature $\theta_D = 140$ K where one speaks of vibrational and librational motions of the whole H_2O molecule instead of translation and rotation.[10] The effective temperature of ^{16}O in water can thus be expressed as

$$T_e = \tfrac{16}{18} T_t + S_r T_t + \frac{1}{6k} \sum_1^3 S_j h \nu_j \left[\frac{1}{e^{h\nu_j/kT} - 1} + \frac{1}{2} \right] , \quad (1)$$

where the first two terms constitute the contribution of the "external" modes of vibration and libration of the H_2O molecule as a whole. The "internal" modes of vibrations are contained in the third term where the factor $\frac{1}{2}$ expresses the contribution of the zero-point vibrational motion which is largely responsible for the higher value of T_e. The above expression is obtained in a similar manner to that explained in detail in Ref. 4 for the case of the NO_3^- molecule. Here, also, the first term expresses the contribution of the translational energy of the O atom and is obtained from that of the H_2O molecule by multiplying by the mass ratio. The second term is the contribution of the rotational-librational motion of the whole H_2O molecule to the kinetic energy of the O atom, where $S_r = 0.149$ is the calculated fraction of the ^{16}O kinetic energy in this motion. The influence of the H bonds and the effect of the surrounding H_2O molecules in water

on both the translational and rotational motions was accounted for by using an effective temperature T_t calculated from the Lamb formula[6] with $\theta_D = 140$ K. The frequencies $\nu_j (j = 1, 2, 3)$ are the three internal modes of vibrations of the H_2O molecule corresponding to one bending mode, a symmetric and an asymmetric stretching mode.[11] In the vapor phase, the H_2O molecule is known to form a triangle with H-O-H angle of $\sim 105°$ having three discrete and well-defined frequencies. In the liquid phase, the distortion by neighboring molecules due to hydrogen bonds causes a large broadening of all modes and a shift of the stretching modes towards lower frequencies and of the bending modes towards higher frequency.[9] The net effect is to leave the value of the effective temperature about the same. Thus, to simplify the problem, we used the normal frequencies for an unperturbed H_2O molecule (in a vapor form) which are listed in Table I. The table also lists the calculated fraction S_j of the kinetic energy shared by the O atom in H_2O, as obtained using standard methods of molecular spectroscopy.[11] In this latter calculation, the H-O-H angle of liquid H_2O was taken as 104.5° and the O-H distance as 0.958 Å which are the parameters for the H_2O molecules in a vapor form.[11]

A bremsstrahlung source, obtained by an electron beam hitting a 100 mg/cm² gold radiator, was used for photoexciting the ^{16}O levels. The electron beam, $E_e = 9.3$ MeV and ~ 10 μA, was obtained from the MUSL-2 accelerator of the University of Illinois having a 100% duty cycle. The experimental system differed from that described in Ref. 12 only in the use of a 5 cm borated plastic shield (against fast neutrons) which greatly reduced the background measured by the 50 cm³ Ge(Li) detector. A photon hardener consisting of bismuth (30 g/cm²), zinc (16 g/cm²), and borated plastic (5 cm), placed in front of the detector was used. The target consisted of 405 g of distilled water placed inside a sealed 10×10 cm² square-shaped styrofoam container. For self-absorption measurements two water absorbers of different thicknesses were used and the comparative nonresonant absorbers consisted of a combination of carbon and aluminum.

A typical scattered spectrum from an H_2O target for an electron beam energy of $E_e = 9.3$ MeV is given in Fig. 1 which shows the two elastic lines at 6.917 and 7.117 MeV obtained using a 4.05 g/cm² target with the Ge(Li) detector at an angle of 90° relative to the incident photon beam. The self-absorption effect of the 6.917 MeV level obtained using a 10.1 g/cm² water absorber was $(27.4 \pm 1.7)\%$. Another absorber, 20.8 g/cm² thick was used and the average of two separate self-absorption measurements was $(44.7 \pm 1.7)\%$. The radiative width obtained from the weighted average of the above measurements was
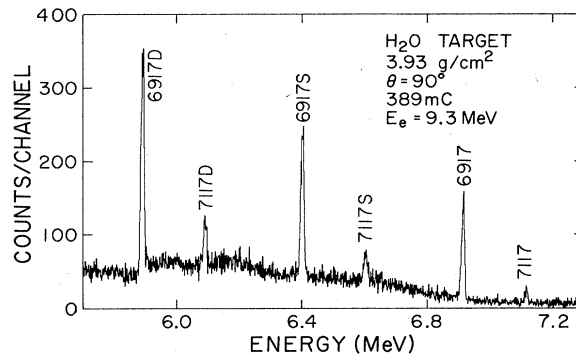

FIG. 1. Typical spectrum obtained using 9.3 MeV bremsstrahlung scattered from an ^1O target in the form of water (H_2O) as measured using a 50 cm³ Ge(Li) detector. A total charge of 389 mC was deposited on the bremsstrahlung radiator during a running time of ~ 10 h. S and D refer to single and double escape peaks, respectively.

$\Gamma_0 (6.917) = 0.091 \pm 0.05$ eV where the following parameters were used: $\Gamma_0/\Gamma = 1$, $J(6.917) = 2$, and the effective temperature of ^{16}O in H_2O at room temperature $T_e(^{16}O) = 410$ K (see above). Another determination of the width of this level using the scattering method is described below. The self-absorption effect of the 7.12 MeV level was small and no attempt was made to carry out a precise determination of its width using self-absorption. Instead, a measurement of the scattering intensity from this level was carried out. Here, the procedure is to determine the curve of the flux-efficiency product $N(E)\epsilon(E)$ for $E > 5$ MeV. This product was obtained for an electron beam energy $E_e = 9.3$ MeV by measuring the scattering intensities from calibration levels in ^{11}B, ^{23}Na, ^{27}Al, and ^{31}P whose widths are well known.[5,13,14] A smooth curve was drawn through the experimental points using a least squares procedure. This curve was used for deducing the values of Γ_0 from the measured scattered intensities from both the 6.917 and 7.117 MeV levels in ^{16}O. The average of three separate determinations were 0.099 ± 0.007 and 0.054 ± 0.004 eV, respectively. The weighted average of the values obtained by the two methods for the 6.917 MeV level is $\Gamma_0 = 0.094 \pm 0.004$ eV. The fact that two different methods yielded relatively close values of Γ_0 for the 6.92 MeV level provides a nice confirmation of the correctness of the calculated value of T_e because the Γ_0 value obtained by the scattering method is almost independent on T_e for relatively thin scatterers. The

TABLE I. Normal frequencies of the H_2O molecule in the vapor phase (in units of cm⁻¹), taken from Ref. 11, and the calculated fraction S_j of the kinetic energy of the ^{16}O atom in H_2O.

Frequency	H_2O (cm⁻¹)	S_j (^{16}O)
ν_1	1595	0.0731
ν_2	3659	0.0727
ν_3	3756	0.0388

TABLE II. Radiative widths in ^{16}O.

	Γ_0 (10^{-3} eV)		Method
	6.917 MeV	7.117 MeV	
Present	94 ± 4	54 ± 4	(γ, γ)
Reference 8	110 ± 5	62 ± 5	(γ, γ)
Reference 15	100 ± 4	$\cdots$	(e, e')
Reference 16	93 ± 10	46 ± 23	(e, e')
Reference 17	80 ± 7	47 ± 6	(γ, γ)
Reference 2	68	$\cdots$	Theory
Reference 3		58	Theory

results of this work are listed in Table II along with previously reported values. It is of interest to note that the present results are in excellent agreement with the average obtained from inelastic electron scattering.[15,16] In addition, our results are close to the average of the values obtained by Swann[4] and Evers et al.,[17] who used the NRF scattering technique. Thus the present values are very close to the adopted values of Ref. 1, being $\Gamma_0 = 0.100 \pm 0.004$ eV and 0.057 ± 0.006 eV for the 6.917 and 7.117 MeV levels, respectively. Further, the value of Swann[4] which is also an average of a scattering and a self-absorption measurement is larger by about 15% than our value. This discrepancy is accentuated even further if one bears in mind that Swann[8]

used a value $T_e = 300$ K (instead of the present value $T_e = 410$ K) in evaluating his self-absorption data. Apparently, this large discrepancy is due to the fact that our measured nuclear absorption is smaller on the average by about 30% than that of Swann.[4] No reason can be invoked to account for such a large difference.

The theoretical predictions[2,3] for the widths of the two levels are also listed in Table II and are of about the same magnitude as that of the measured values.

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