LEVEL ENERGIES AND INFRARED RADIATIVE LIFETIMES OF THE MUONIC MOLECULE Heμ+

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Energies and radiative lifetimes are calculated for all bound and quasibound levels of the positive muon molecular ion Heμ+, together with the tunneling predissociation lifetimes of its quasibound levels. The radiative lifetimes obtained are much longer than the positive muon decay lifetime, so spontaneous ("infrared") emission will not be a useful diagnostic for the presence of Heμ+ or the analogous molecular ions formed by the heavier inert gas atoms.

1. Introduction

With its charge of +e and mass of approximately $\frac{1}{9}$ u, the positive muon μ^+ is expected to behave chemically (insofar as its lifetime allows it) as the nucleus of an atom of a particularly light isotope of hydrogen. As a result, all ionic chemical species formed by protons may be expected to have positive muon analogues. Since inert gases are often used as the target material in the meson experiments in which muons are thermalized and muonium is produced, the muon analogues of the inert gas hydride molecular ions are clearly species which can be expected to be observed. Indeed, observations of Heμ+, Neμ+ and probably also Arμ+ have already been reported [1–3].

A previous communication from this laboratory [4] reported values of the energies of all bound and quasibound vibration–rotation levels and the tunneling predissociation lifetimes of the quasibound levels of the ground electronic states of Heμ+ and Neμ+, all calculated from the best available potential energy curves [5–8]. These results are of interest because a knowledge of such energies could facilitate the experimental identification of positive muon molecular ions, while a

knowledge of the properties of their quasibound levels should help predict the probability of forming them. This previous paper also reported a radiative lifetime calculated for one of the possible spontaneous infrared transitions of Heμ+.

The present paper extends the calculations of ref. [4] in two ways: (i) the predictions regarding the properties of quasibound levels are extended to include shape resonances lying above the (centrifugal) potential energy barriers, and (ii) radiative lifetimes are reported for all bound and quasibound levels of Heμ+. The latter results should answer the question of whether these species may be observed via their spontaneous "infrared" emission spectra. Comparisons of the dipole moment function of Heμ+ with those of other inert gas–positive muon molecular ions should indicate whether this might be possible for them too.

2. Potential energy curve and computationsl methods

The potential energy curve for Heμ+ used in the present work is exactly the same adiabatically corrected potential used to produce the results in table 4 of ref. [4]. It was generated by combining the "clamped nuclei" Born–Oppenheimer potential for HeH+ reported by Kołos and Peek [5] with the appropriately mass-weighted adiabatic corrections calculated by Bishop and Cheung [6]. Beyond the range of the ab initio

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points, the potential was extrapolated as a sum of inverse power terms $C_4/r^4 + C_6/r^6 + C_8/r^8$, where the coefficients were determined by a fit to the last three numerical potential points.

The accuracy of such a calculation is limited by the accuracy of both the ab initio points themselves and of the interpolation procedure used with them. In the present work, this interpolation was done using 4-point pievewise Lagrangian polynomials. Tests with a variety of other interpolation schemes suggest that "interpolation noise" is responsible for eigenvalue uncertainties ranging from ≈ 0.1 cm^{-1} for the highest levels to 1 cm^{-1} for the most strongly bound ones. The only way this uncertainty could be reliably reduced would be if the ab initio points were calculated to higher accuracy and on a denser mesh.

The eigenvalues and eigenfunctions of the bound and quasibound levels were calculated by a standard numerical procedure based on the Cooley–Cashion application of the Numerov algorithm [9–13]. The quasibound levels lying above the dissociation limit but below the centrifugal potential barrier maxima were located using both the Airy function boundary condition and collisional time delay methods of refs. [12,13], while the latter approach was used to calculate the properties of the orbiting resonance levels lying above these centrifugal barrier maxima. The overlap integrals between pairs of radial wavefunctions required for calculating radiative lifetimes were evaluated by Simpson's rule. In all of these calculations, the values of the physical constants were introduced via the single factor [14] $\hbar^2/2m = 16.857630/m$ cm^{-1} Å^2, where $m = 0.11030250$ u is the He–μ^+ reduced mass.

3. Results for the ground state of Heμ^+

3.1. Level energies and widths

The energies of all bound levels and of those orbiting resonance levels of Heμ^+ lying below centrifugal barrier maxima are listed in table 1. These results are essentially identical to those reported in table 4 of ref. [4], except that one additional quasibound level (one lying above dissociation but below a barrier maximum), $(v,j) = (1,7)$, is included here. The only apparent discrepancies with ref. [4] (other than correction of a typographical error for the ground state) occur for the (v,j)

Table 1
Bound and quasibound level energies of Heμ^+ (in cm^{-1}) calculated from the adiabatically-corrected Born–Oppenheimer potential. The zero of energy lies at the dissociation limit

j	$v = 0$	$v = 1$	$v = 2$	$v = 3$
0	−12255.5	−5849.0	−1766.7	−134.2
1	−11804.9	−5508.4	−1551.4	−69.6
2	−10923.6	−4847.1	−1145.0	13.9
3	−9650.0	−3904.3	−599.6	
4	−8038.7	−2738.2	−12.4	
5	−6157.6	−1427.9		
6	−4086.5	−87.2		
7	−1917.3	1050.6		
8	235.1			
9	2160.4			

$= (0,9)$ and $(3,2)$ quasibound levels, which are predicted to lie, respectively, 8 and 3 cm^{-1} lower than was reported previously [4]. These differences reflect the present preference for level energy predictions yielded by quantum mechanical time delay calculations [12,13], over those yielded by the Airy-function boundary condition method [12] used exclusively in ref. [4]. For the first of these levels, this difference is only a few percent of the magnitude of the level width, and hence is too small to have any physical significance [12,13]. For the other, $(v = 3, j = 2)$, the corresponding difference is almost half of the level width, an unusually large error. This serves as a reminder that the Airy function boundary condition method [12] is, after all, an approximate procedure, and that the situations in which its weakness is most likely to appear are those in which the potential barrier is very asymmetric and the tunneling rate is high.

Table 2 lists the energy, the full-width at half-maximum Γ, and the "tunneling predissociation" lifetime τ_t for all of the quasibound levels of table 1, as well as for the first orbiting resonance level for each v which lies above the appropriate centrifugal barrier maximum. All these results were calculated quantum mechanically from the corresponding collisional time delay functions [12,13]. Although only the highest j level listed for each v lies above the centrifugal potential barrier, all but $(v,j) = (0,8)$ and perhaps also $(3,2)$ are sufficiently broad that they cannot be expected to be observed as discrete structure in an optical spectroscopic experiment.

Table 2

Collisional time delay predictions of the energies E, widths Γ and "tunneling" predissociation lifetimes τ_t for quasibound and orbiting resonance levels of $He\mu^+$

v	j	E (cm^{-1})	Γ (cm^{-1})	τ_t (s)
0	8	235.1	0.15×10^{-4}	3.51×10^{-7}
0	9	2160	100	5.31×10^{-14}
0	10	3831	852	6.23×10^{-15}
1	7	1051	160	3.32×10^{-14}
1	8	1984	1160	4.57×10^{-15}
2	5	426	251	2.12×10^{-14}
3	2	13.9	8.0	6.60×10^{-13}
3	3	68.9	203	2.61×10^{-14}

Table 3

Radiative lifetimes (in μs) for all the bound and quasibound levels of $He\mu^+$

j	$v = 0$	$v = 1$	$v = 2$	$v = 3$
0	–	36	40	183
1	25296	38	44	265
2	2710	42	54	1758
3	786	49	77	
4	342	60	153	
5	188	77		
6	120	106		
7	87	214		
8	72			
9	76			

3.2. Infrared radiative lifetimes

For all of the bound and quasibound levels of ground state $He\mu^+$, we have calculated the Einstein A coefficients for spontaneous emission to all lower levels accessible via the normal infrared selection rule $\Delta j = \pm 1$. These values were generated from the usual expression:

$$A = 3.1361 \times 10^{-7} \, S(j',j'')\nu^3 \, |\langle\psi_i|M(r)|\psi_j\rangle|^2, \qquad (1)$$

where A is in s^{-1}, $M(r)$ the dipole moment function (in debye), v the level spacing in cm^{-1}, $S(j',j'')$ the rotational intensity factor, and ψ_i and ψ_j are the unit normalized initial and final state radial wavefunctions. For the present case of transitions among levels of a $^1\Sigma$ state, $S(j',j'')$ has the values max$(j',j'')/(2j'+1)$, where j' and j'' are the rotational quantum numbers of the initial (emitting) and final levels. The dipole moment function used here is that suggested by Dabrowski and Herzberg [15]: $M(r) = 1.66 + 3.22(r - r_e)/r_e$ debye, distances are in ångstrom and $r_e = 0.77436$ Å.

Ref. [4] reported an A factor or radiative lifetime for the single transition $(v = 0, j = 8) \rightarrow (0,9)$. However, the result given there was in error by an order of magnitude. The correct A coefficient and radiative lifetime τ_r associated with this transition are: $A = 1.39 \times 10^4$ s^{-1} and $\tau_r = 72 \mu$s.

Table 3 summarizes the results of the present lifetime calculations. For $v = 0$ levels, the only possible transitions are $\Delta v = 0$ and $\Delta j = -1$, while for vibrationally excited levels the tabulated radiative lifetimes also include contributions from $\Delta j = \pm 1$ for all possible (negative) values of Δv. It is interesting to note that

for all the $\Delta v = 0$ transitions, and for many of those for $\Delta v < 0$, the linear and constant terms in the dipole moment function make comparable contributions to the overall matrix elements.

4. Discussion and conclusions

Unfortunately, all of the radiative lifetimes shown in table 3 are significantly longer than the 2.2 μs decay lifetime of the positive muon. It therefore appears that infrared emission will not be a useful diagnostic for the presence of $He\mu^+$.

Without undertaking detailed calculations, one may readily predict that this type of emission is also unobservable for other inert gas—positive muon molecular ions. If the dipole moments of these species are written in the form

$$M(r) = a_0 + a_1(r - r_e)/r_e, \qquad (2)$$

where r_e is the equilibrium distance, the values of the coefficients a_0 and a_1 for $Ne\mu^+$, $Ar\mu^+$ and $Kr\mu^+$ are all positive and lie within a factor of 2 of the corresponding $He\mu^+$ constants [16,17]. Corresponding states arguments suggest that the radial overlap integrals should be fairly similar for all these systems. The infrared emission lifetimes of molecular ions formed between μ^+ and the heavier inert gas atoms will therefore also be much longer than the positive muon decay lifetime, so such emission will be no more useful for observing them than it was for $He\mu^+$.

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