Calculation of structures and transition rates of muonic molecular ion H_2Mu^+

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A muonic molecular ion H_2Mu^+ consists of a positive muon, two protons and two electrons. The existence of H_2Mu^+ was suggested by analyzing the μSR (Muon Spin Relaxation) signals, injecting muons into the solid hydrogen target [1]. Belov *et al.* calculated the lifetimes of excited states of H_2Mu^+ for $J = 0 \sim 2$ (J is the total angular momentum of H_2Mu^+) with the conventional method of molecular dynamics [2]. To investigate the formation and cascade process of H_2Mu^+, we calculated not only low-lying rotational-vibrational states but also highly excited states ($J \leq 6$, $v \leq 15$).

The electronic motion can be separated from that of the muon and proton motion in adiabatic approximation because the mass of an electron is much smaller than that of a muon and a proton. We treated H_2Mu^+ as a three-body system on the adiabatic potential surface due to the electronic motion. The potential energies of H_2Mu^+ in the ground electronic state $^1A'$ was calculated by a full configuration interaction (CI) treatment with a [8s6p2d1f] Gaussian-type basis set [3].

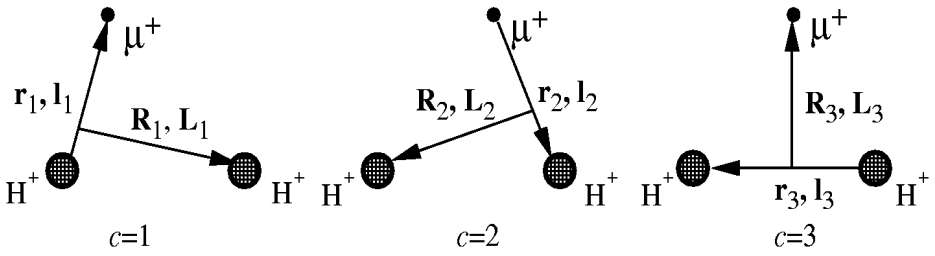

Figure 1: Three rearrangement Jacobian coordinates of three-body system.

The total energies and wave functions of the three-body system were calculated with a coupled rearrangement channel method [4]. The total three-body wave function Ψ^{tot}_{JMv} is described as a sum of the three rearrangement channel amplitudes,

$$\Psi^{tot}_{JMv} = \sum_{c=1}^{3} \sum_{\ell_c L_c n N} A^{(c)Jv}_{\ell_c L_c n N} r_c^{\ell_c} R_c^{L_c} \exp\left(-\frac{r_c^2}{\nu_n^2} - \frac{R_c^2}{\lambda_N^2}\right) \left[Y_{\ell_c}(\hat{\mathbf{r}}_c) \otimes Y_{L_c}(\hat{\mathbf{R}}_c)\right]_{JM}, \qquad (1)$$

where M is projection of J on z-axis and v is the number of nodes of the wave function. The Gaussian range parameters ν_n and λ_N are taken to be a geometrical progression. Each channel

amplitude is described by the coordinates in Fig. 1. The coordinates $c = 1$ and $c = 2$ are suited for describing the HMu + H^+ configuration. The coordinate $c = 3$ is suited for describing the $H_2 + \mu^+$ configuration. The electric dipole transition ($E1$) rates λ_i of the rotational-vibrational states of H_2Mu^+ were calculated with

$$\lambda_i^{E1} = \sum_f \frac{4(E_f - E_i)^3}{3\hbar^4 c^3} \left| \left\langle \Psi_i^{tot} \right| \mathbf{d} \left| \Psi_f^{tot} \right\rangle \right|^2, \tag{2}$$

where Ψ_i^{tot} and Ψ_f^{tot} are the total wave functions of initial and final states. The values E_i and E_f are the total energies of initial and final states. The vector $\mathbf{d}$ is the dipole moment of H_2Mu^+.

The binding energies ε respected to the lowest two-body break-up threshold $H_2 + \mu^+$ (H^+), the mean distances r_{ij} between the constituent particles (i, j) and the $E1$ transition rates λ^{E1} of states of H_2Mu^+ and H_3^+ are listed in Table 1, for example. Since the adiabatic potential is independent of the mass of the three particles the molecular ion H_2Mu^+ is expected to be analogous to H_3^+, but the energy and structure are different from H_3^+. The structure of H_2Mu^+ and H_3^+ in the ground state are an isosceles triangle and an equilateral triangle, respectively. Because a muon is lighter than a proton, the binding energy of muon in H_2Mu^+ is smaller than the proton in H_3^+. Therefore the distance $r_{p\mu}$ in H_2Mu^+ is longer than the distance r_{pp} in H_3^+. While the distance r_{pp} in H_2Mu^+ is shorter than the distance r_{pp} in H_3^+, because an electron density in the sub-system H_2 of H_2Mu^+ is higher than that of H_3^+.

The $E1$ transition rates of the excited states are smaller than the decay rate of muon (0.455 μs^{-1}). The molecular ion H_2Mu^+ formed in highly excited states can not reach the ground state within the lifetimes of muon.

Table 1: Binding energies ε respected to two-body break-up threshold $H_2 + \mu^+$ (H^+), mean distances $r_{p\mu}$ between muon and proton, and mean distances r_{pp} between two protons and lifetimes of states $({}^{2s+1}J_v^\pi)$ of H_2Mu^+ and H_3^+. (s is the total spin of two protons, π is the parity of the wave function.)

system	states $({}^{2s+1}J_v^\pi)$	ε (au)	$r_{p\mu}$ (au)	r_{pp} (au)	λ^{E1} (s^{-1})
H_2Mu^+	${}^1 0_0^+$	0.1461	1.812	1.717	0
H_3^+	${}^1 0_0^+$	0.1608		1.722	0
H_2Mu^+	${}^1 0_5^+$	0.1095	1.860	2.202	4.0×10^3
H_2Mu^+	${}^1 5_0^+$	0.1368	1.843	1.741	1.3×10^1

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