AL-AZHAR BULLETIN OF SCIENCE

Bulletin of Faculty of Science Al-Azhar University

ISSN 1110-2535

Vol. 9, No. 2 *(Dec.) 1998*

Al-Azhar Bull. Sci. Vol. 9, No. 2 (Dec.) : pp 1055- 1065, 1998.

CHEMICAL REACTION OF μ^+ MESONS WITH HYDROGEN MOLECULAR IONS

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Abstract

The zero order cross sections for the chemical reaction of (μ^+) mesons with hydrogen molecular ions have been calculated neglecting its radioactive character.

A modified form for the cross-section of the reaction $\mu^+ + H^+_2 \rightarrow (\mu H)^+ + H^+$ is derived. The differential cross-sections for different excited state of the above reaction has been calculated using the suggested form. The wave functions for the relative motion of (μ^+) mesons in the field of (H^+_2) and hydrogen ion in the field of $(\mu H)^+$ has been calculated using the "NEWMAN - THORSON" modified method.

Introduction

The problem of scattering of (μ^+) mesons with molecules has been the focus of interest of scientists. In the presence of matter, (μ^+) mesons will undergo chemical reaction which may depolarize matter. The extent of this depolarization may be determined by the change in the angular correlation with the emission of position in the decay process.

In a previous work (Ayob 1969) an expression for the differential cross-section for the collision of nucleons with (μ^+) mesons was derived. The method of calculation was proposed (Massey 1949) and further developed by (Ayob 1982). In this work the two particular solutions for the schrödinger equation and the algebralically related quantities are completely smooth nonoscillatory functions with variations controlled only by those of the classical Hamiltonian function.

A method for calculating the differential cross-section of scatering of (μ^+) meson by hydrogen molecular ion is proposed as a modification for the method used by NEWMAN and THORSON (1972).

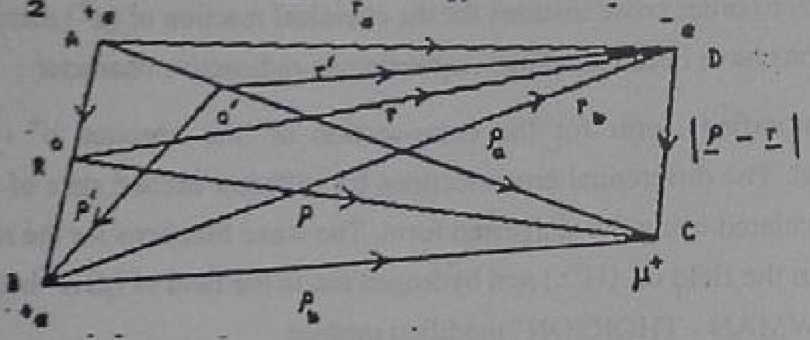
The aim of this paper is to study theoretically the rate of chemical reactions of mesons with hydrogen molecular ions.

The cross-section is derived in the frame-work of the distorted wave approximation for a collision in which (μ^+) mesons is incident on $(H^2{}_1)_2$ resulting in a rearrangement in which (μ^+) is captured and ($H^2{}_1$) is leaving ($\mu H^2{}_1$).

The modified formulation of the problem:

We consider the reaction

$$\mu^+ + H_2^+ \longrightarrow (\mu H)^+_{r_a} + H^+$$



the wave equation for the complete system may be written either in terms of the initial state:

$$\left[H(r,R) - \frac{h^2}{8\pi^2 M}\nabla^2_\rho + e^2\left(\frac{1}{\rho_b} + \frac{1}{\rho_a} - \frac{1}{|\rho - r|}\right) - E\right]\psi = 0 \tag{1}$$

or in terms of the final state:

$$\left[H'(r,\rho_a) - \frac{h^2}{8\pi^2 M_2}\nabla^2_{\rho'} + e^2\left(\frac{1}{R} + \frac{1}{\rho_b} - \frac{1}{r_b}\right) - E\right]\psi = 0 \tag{2}$$

where H & H^1 are the Hamiltonians for the internal motion of ($H^+{}_2$) and (μH) respectively.

M_1, M_2 are the reduced masses of ($H^+{}_2$), (μ^+) and $(\mu H)^+$, (H^+) respectively

$$\underline{\rho} = \frac{1}{2}\left[\frac{2M + \mu}{M + \mu}\underline{\rho}_a - \underline{\rho}'\right]$$

represent the vector separation between (μ^+) and the center of mass of ($H^+{}_2$), where M, μ are the masses of proton and (μ^+) meson respectively.

Also the vector separation between H^+, and the center of mass of $(\mu H)^+$ is

$$\rho' = \frac{M}{M+\mu}\, \rho_a - \rho_b$$

Also $$E = E_{H_2} + \frac{h^2}{8\pi^2 M_1} K_1^2 = E_{(\mu H)^+} + \frac{h^2}{8\pi^2 M_2} K_2^2$$

where K_1, K_2 are the wave numbers of the relative motion of (μ^+) and (H^+) respectively. We now approximate ψ, the wave function representing the whole system, in the form

$$\Psi = \psi\,(r,R)\,\chi(R)\,F(\rho) + \phi\,(r,\rho_a)\,\Omega(\rho_a)\,G\,(\rho') \qquad (3)$$

where ψ, ϕ are the wave functions of the electron in the field of the two proton at A, B and proton at A, (μ^+) respectively. Thus, we may write

$$\psi = [\,N(R)\,]\,[\,e^{-\alpha r_{-a}} + e^{-\alpha r_{-b}}\,] \qquad (4)$$

$$\phi = [\,N(\rho_a)\,]\,[\,e^{-\alpha r_{-a} - \rho_a)} - e^{-a\rho_a}\,] \qquad (5)$$

where $N(R) = \sqrt{\dfrac{\alpha^3}{2L + g(R)}}$, $N(\rho_a) = \sqrt{\dfrac{\alpha^3}{2L + g(\rho_a)}}$

$$\alpha = a_o^{-1} \text{ and } g(\rho) = e^{-a\rho}\left(1 + a\rho + \frac{\alpha^2 \rho^2}{3}\right)$$

The vibrational wave functions for the ground state of $(H^2_1)_2$ and (μH^2_1) molecules which are $\chi(R)$ and $\Omega\,(\rho_a)$ are taken as

$$\chi\,(R) = N\,(R)\,e^{-a_1/2\,(R-R_o)^2} \qquad (6)$$

$$\Omega\,(\rho) = N\,(\rho_a)\,e^{-a_2/2\,(\rho_a-\rho_{a_o})^2} \qquad (7)$$

where

$$N(R) = \frac{a_1^{1/4}}{2\pi^{3/4}\,R_o} \quad \text{and} \quad N(\rho_o) = \frac{a_2^{1/4}}{2\pi^{3/4}\,\rho_{ao}}$$

Finally the wave functions $F(\rho)$ and $G(\rho')$ for the relative motion of (μ^+) mesons in the field of $(H^2_1)_2$ and Hydrogen ion in the field of (μH^2_1) respectively are the solutions of the following equations

$$\left[\nabla_\rho^2 + K_1^2 - \left(\frac{2M_1}{h} \right) V_1 \right] F = 0 \tag{8}$$

$$\left[\nabla_{\rho'}^2 + K_2^2 - \left(\frac{2M_2}{h} \right) V_2 \right] G = 0 \tag{9}$$

Where V_1 and V_2 are the mean interaction energies of (μ^+) meson with Hydrogen molecular ion and Hydrogen ion with (μH^2_1) respectively.

Now for the internal motion we have

$$\left[H \;(r, \rho) - E_{H_2} \right] \psi\,(r, R)\; \chi\,(R) = 0 \tag{10}$$

$$\left[H'(r', \rho_a) - E_{(\mu H)^+} \right] \phi\,(r', \rho)\; \Omega\,(\rho_a) = 0 \tag{11}$$

Subituting (3) into (1) using (10), multiplying by ψ, χ, integrating over the space of χ, R, and using the normalizing condtion.

$$\int |\psi|^2 \, |\chi|^2 \, dr \, dR = 1$$

the wave equations (1), (2) for the complete system may be written either in terms of the initial state

$$\left[\nabla_\rho^2 + K_1^2 - \frac{8\pi^2 M_1}{h^2} V_1 \right] F = \frac{8\pi^2 M_1}{h^2} \int \psi \chi \Big[- V_2 + e^2 \left(\frac{1}{\rho_b} + \frac{1}{R} - \frac{1}{r_b} \right) \phi \, \Omega \, G_0 \, dr \, dR \tag{12}$$

or in terms of final state, i.e.

$$\left[\nabla_{\rho'}^2 + K_2^2 - \frac{8\pi^2 M_2}{h^2} V_2 \right] G = \frac{8\pi^2 M_2}{h^2} \int \phi \, \Omega \Big[- V_1 + e^2 \left(\frac{1}{\rho_a} + \frac{1}{\rho_b} - \frac{1}{|\varrho - r|} \right) \Big] \psi \chi \, F_0 \, dr' \, d\varrho_a \tag{13}$$

$$V_1 = e^2 \int \left(\frac{1}{\rho_a} + \frac{1}{\rho_b} - \frac{1}{|\rho - r|} \right) |\psi|^2 \, |\chi|^2 \, dr \, dR \qquad (14)$$

$$V_2 = e^2 \int \left(\frac{1}{R} + \frac{1}{\rho_b} - \frac{1}{r_b} \right) |\phi|^2 \, |\Omega|^2 \, dr' \, d\rho_a \qquad (15)$$

M_1, M_2 are the reduced masses of (H_2^+, μ^+) and $((\mu H)^+, H^+)$ respectively.

On treating the R-H-S of equation (2) as a known function (Ayob 1982), we have the asymptotic form of G.

$$\left[\nabla^2_{\rho'} + K_2^2 - \frac{8\pi^2 M_2}{h^2} V_2 \right] G = \frac{8\pi^2 M_2}{h^2} \int \phi \, \Omega \, G_o \Big[-V_1 +$$

$$e^2 \left(\frac{1}{\rho_a} + \frac{1}{\rho_b} - \frac{1}{|\rho - r|} \right) \Big] \psi \, \chi \, F_o \, dr \, d\rho'_a \, d\rho' \qquad (16)$$

where G is the solution of the homogeneous equation

$$\left[\nabla^2_{\rho'} + K^2_2 - \frac{8\pi^2 M_2}{h^2} V \right] G_o = 0 \qquad (17)$$

In (Ayob. 1969) the first term on the right hand side of the equation (13) is neglected.

In the present work, we are going to deal with the general solution which has the function (Ayob 1982).

$$G \sim \left(\frac{8\pi^2 M_2}{h^2} \right) \left(\frac{i_e k\rho'}{\rho'} \right) \left(\frac{-1}{4\pi} \right) \int \phi \, \Omega \, G_o \Big[-V_1$$

$$+ e^2 \left[\frac{1}{\rho_a} + \frac{1}{\rho_b} - \frac{1}{(\rho - r)} \right] \Big] \psi \, \chi \, F_o \, d\, r' \, d\rho_a \, d\rho' \qquad (18)$$

For this, the differential cross-section for the transition from the initial state to the final state will be

$$Q = \frac{M_1 M_2}{\pi a_o^2} \frac{K_2}{K_1} |I|^2 \tag{19}$$

$$\text{where } I = \int \psi \chi F_o \left[-V_1 + e^2 \left(\frac{1}{\rho_a} + \frac{1}{\rho_b} - \frac{1}{(\underline{\rho} - \underline{r})} \right) \right] \varphi \; \Omega G_o \; d\underline{r}' \; d\rho_a \; d\underline{\rho}' \tag{20}$$

and K_1, K_2 are the wave numbers of the incident (μ^+) and scattered (H^+) respectively. Now we consider the interaction V_1 in the form

$$V_1 = e^2 \int \frac{1}{\rho_a} + \int \frac{|\chi(R)|^2}{\rho_b} d\underline{R} - \frac{1}{|\underline{\rho} - \underline{r}|} |\psi|^2 |\chi|^2 \, d\underline{r} \, d\underline{R} \tag{21}$$

The third term on the R.H.S. of (21) rpresents the interaction bwtween the electron and the μ^+ meson. It can be neglected in comparison with the interaction between the proton and the μ^+ meson since these particles do not form a bound state in this reaction under consideration. Thus we may write.

$$V_1 = e^2 \left[\frac{1}{\rho_a} + NJ \right] \tag{22}$$

where $N = \dfrac{a_1}{4\pi^{3/2} R_o^2}$ and

$$J = \int \frac{1}{\rho_b} e^{-a(R-R_o)^2} dR \tag{23}$$

By using the elliptic coordinates

$$\lambda = \frac{\rho_b + R}{\rho_a}, \quad \mu = \frac{\rho_b - R}{\rho_a},$$

the quantity (J) takes the form

$$J = \frac{\pi}{4} \rho_a^3 \int_{-1}^{1} \int_{1}^{\infty} \exp\left\{ -\alpha_1 \left[\frac{1}{2} \rho_a (\lambda - \mu) - R_o \right]^2 \right\} (\lambda - \mu) \, d\lambda \, d\mu \tag{24}$$

We carry out the above integration by expanding it in values of λ, μ, $\rho\mu_b$, R_o to attain

$$J = \frac{\pi R_o \rho_a^2}{2}\left[\sqrt{\frac{\pi}{C_1}} - \frac{1}{C_1}\sum_{k=o}^{\infty}(-1)^{k+1}\frac{(\sqrt{C_1})^{2k+1}}{2k\ (2k-1)(k-1)!}\right.$$

$$\left.\left\{(C_2+1)^{2k}-(C_2-1)^{2k}\right\}\right] + \frac{1}{2(C_1)^{3/2}}\sum_{k=o}^{\infty}\frac{(-1)^{k+1}(\sqrt{C_1})^{2k-1}}{(2k-1)\ (k-3)!}$$

$$\left[(C_2+1)^{2k-1} - (C_2-1)^{2k-1}\right] \qquad (25)$$

where $C_1 = \frac{a_1 \rho_a'}{4}$ and $C_2 = \frac{2R_o}{\rho_a}$

Using (22) into (20)

$$I = e^2 \int \psi\, \chi\, F_o\left[\frac{1}{\rho_b} - NJ - \frac{1}{|\underline{\rho} - \underline{R}|}\right]\phi\Omega\ G_o\ d\underline{r}'\ d\rho\ d\underline{\rho}' \qquad (26)$$

Method of calculation:

The distorted wave approximation in which the rearrangment is taken into account approximates y in the form (3), where ψ, ϕ can be obtained from the equations (4), (5) respectively and χ, Ω can be obtained from (6), (7) respectively, and to get F, g we shall solve the equations (8), (9) using the semiclassical approximation.

For this purpose we consider the following functions

$$\psi_{\pm}(X) = \exp \pm \frac{iS(X)}{h} \qquad (27)$$

where the complex function S (X) is smoothy is smppthly varying. We assume that these function are solutions of the following equation

$$\frac{d^2\psi}{dX^2} + K^2(X)\ \psi = 0 \tag{28}$$

With classical part $K^2(X)$ where

$$K^2(X) = \frac{8m\pi^2}{h^2}\left[E - V(X)\right]$$

We search for the solution in the form

$$\psi(X) = a_+(X)\ w_+(X) + a_-(X)\ w_-(X) \tag{29}$$

where

$$W_{\pm}(X) = \exp \pm i \int_{X_o}^{X} K\,(X')\ dX'$$

and X_o is any conveniet reference point. Substituting (29) in (28) and taking into consideration the variation of constants constraint,

$$a'_+(X)\ w_+(X) + a'_-(X)\ w_-(X) = 0,$$

we get the solution in the form

$$\psi_{\pm}\ (X) = C_o \exp \pm i \int_{X_o}^{X} K(X')\ \frac{1 - \phi\ (X')}{1 + \phi\ (X')}\ dX' \tag{30}$$

where C_o is constant, ϕ has the first approximation

$$\phi_o(X) = -ik'\,(X)\ /\ 4k^2(X),$$

This result is then substituted into the right hand side of the equation

$$\phi(X) = \phi(X)\left[1 - \phi(X)\right] + \frac{i\phi'\,(X)}{2k(X)}$$

A second approximation for ϕ is obtained and the process iterated if possible to convergence.

Substituting ϕ into equation (30), we obtain

$$\psi(X)=C_o \exp i \int_{X_o}^{X} \frac{H_1 D_1 + H_{11} D_{11} + i(H_{11} D_1 + H_1 D_{11})}{D_1^2 + D_{11}^2} dx \tag{31}$$

where

$$D_1 = S_1(X) + \frac{K'(X)}{S_1} (1 + Q_1)^2 - \left(\frac{T_x}{S_x}\right)^2$$

$$D_{11} = \frac{K'(X)}{K(X)} (1+Q_1)\left(\frac{T_x}{S_x}\right)$$

$$H_1 = K(X)\, S_1(X) - \frac{K'^2(X)}{4K(X)} (1 + Q_1)^2$$

$$+ K(X) \left(\frac{T_x}{S_x}\right)^2 - \left(\frac{T_x}{S_1(X)}\right)$$

$$H_{11} = 2\, K(X)\, K'(X)\, (1 + Q_1)$$

$$- K'(X)\, (1 + Q_1)\left(\frac{T_x}{S_x}\right)$$

$$T_x = 4K^2(X)\, K''(X) - 8K(X)\, K'^2(X)$$

$$S_1(X) = 4K^2(X) \;\&\; S_x = S_1^2(X) \;\&\; Q_1 = \frac{K'^2(X)}{S_x} \;\&$$

$$K(X) = \sqrt{\frac{8m\pi^2}{h^2} [E - V(X)]}$$

and V(X) is taken as a Morse potential of the form

$$V(X) = D_o \left[e^{-2a(X-X_o)} - 2\, e^{-a(X-X_o)} \right]$$

Integrating the equation (31), we obtain the wave function ψ, where D_o is the lowest energy value at the equilibrium separation. To a good approximation the potential can be assumed to be infinitely large at $X = X^1 \le 0.3a_o$.

Therefore the wave function will be zero for $X = 3.a_o$, the initial slope was chosen to be 0.00097 under these consideration equation (7) & (8) are solved numerically as we proposed by the modified method of NEWMAN-THORSON.

When the atomic units are introduced, the differential cross-section Q for the transition from the initial state to the final state will be

$$Q = \frac{M_1 \; M_2}{\pi \, m_e^2} \; \frac{K_2}{K_1} \; |I|^2$$

Where m_o is the mass of the electron and I is the integral of the scattered amplitude and is given by

$$I = \int \psi \, \chi \, F \left(\frac{1}{\rho_a} + \frac{1}{\rho_b} + \frac{1}{\rho_o}\right) \phi \, \Omega \, G \, dr' \; d\rho \; d\rho'$$

Results and Discussion

The present calculated values of the differential cross-section and the corresponding theoretical ones are comparable with our calculations give:

K	Q_{cal}	Q_{Max}	$Q_{Max} - Q_{cal}$
5.9324	0.15842	0.16857	0.01015
8.8986	0.11121	0.11238	0.00117
11.8648	0.08362	0.08427	0.000065

1. The differential cross-section for the different energies of the above reaction has been calculated using this method and more accurate results had been obtained.

2. Analytically solvable model problems show that the logarithmic derivation of such solutions can usually be calculated 4-to-8 orders of magnitude more accurate than those which can be obtained by direct numerical integrations of Schrödinger equation and Hence a good result obtained.

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