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CROSS SECTIONS FOR SPIN EXCHANGE COLLISIONS BETWEEN FAST HYDROGEN ATOMS AND HYDROGEN OR ALKALI ATOMS

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Abstract

Spin exchange cross sections have been calculated for hydrogen atoms with energy in the keV range incident on hydrogen or alkali atom targets. The cross sections generally decrease with increasing energy, but also show oscillations as a function of the energy. For a hydrogen atom with an energy of 5 keV incident on a sodium atom target, the total spin exchange cross section is $1.2\times10^{-15}\text{cm}^2$.

There is current interest in the production of polarized hydrogen atoms or ions by capture of a polarized electron as a fast H ion passes through an electron spin polarized atomic target [1-5]. It is possible that spin exchange collisions as well as charge transfer collisions may play a role in these ion sources.

There are previous calculations but no experiments on low energy spin exchange cross sections for H incident on a hydrogen or alkali target [6-9]. This paper presents the first calculations of the spin exchange cross sections for fast H atoms incident with energy in the range 0.1-10 keV on a hydrogen or alkali target. At the present time there are no experimental spin exchange cross sections available in this energy range.

When two atoms, each having electron spin, collide, it is possible for the atoms to undergo spin exchange. Because of the hyperfine structure the details of a spin exchange collision depend on the magnetic field in which the collision occurs. We treat the case of spin exchange in a magnetic field high enough that the electron spin and the nuclear spin of both atoms are decoupled so that the effects of nuclear spin can be ignored. In a spin exchange collision, two atoms, one with electron spin S_1 and z component of electron spin M_1, and the other with electron spin S_2 and z component of spin M_2, collide and emerge with quantum numbers S_1, M_1' and S_2, M_2'. In order to make the discussion concrete we shall initially discuss the collision of a H atom with $M_1 = 1/2$ and a Na atom with $M_2 = -1/2$. Let us also suppose the collision occurs with a given impact parameter b, and energy E. The initial wave function is a linear superposition of the $^1\Sigma$ and $^3\Sigma$ wave functions, which correspond in the separated atom limit to ground level H and Na. Thus the initial wave function of the system can be written as

$$\psi_i = \frac{1}{2}\big(\alpha(1)\beta(2) + \alpha(2)\beta(1)\big)\psi_{3_\Sigma} + \frac{1}{2}\big(\alpha(1)\beta(2)-\alpha(2)\beta(1)\big)\psi_{1_\Sigma} \qquad (1)$$

where α and β are respectively electron spin up and spin down wave functions and ψ_{3_Σ} and ψ_{1_Σ} are respectively the spatial parts of the $^3\Sigma$ and $^1\Sigma$ wave functions. As the atoms collide the triplet part of the wave function is coupled only weakly to excited levels, and we ignore this coupling. The singlet part of the wave function is, however, coupled strongly to excited levels, primarily the $H^- + Na^+$ level, and through this level to the $H + Na(3P)$ level. After the collision the final wave function is represented by

$$\psi_f = \frac{1}{2}\big(\alpha(1)\beta(2) + \alpha(2)\beta(1)\big)\psi_{{}^3\Sigma}\, e^{-i\int V_t dt/\hbar}$$

$$+ \frac{A_1}{2}\big(\alpha(1)\beta(2) - \alpha(2)\beta(1)\big)\psi_{{}^1\Sigma}\, e^{-i\int V_s dt/\hbar} + A_2\psi_{H+Na(3P)} + A_3\psi_{H^-+Na^+} \quad (2)$$

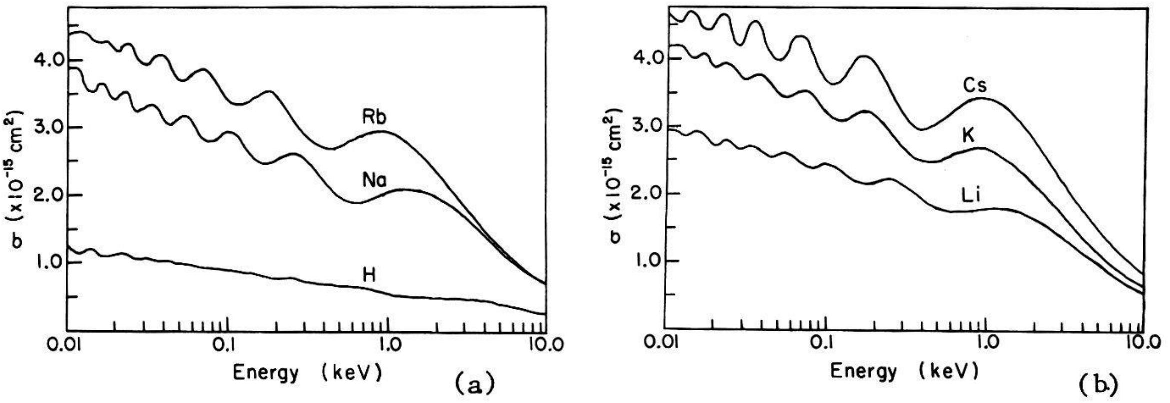
where V_t and V_s are the interaction potentials for the $^3\Sigma$ and $^1\Sigma$ levels and where $A_1/\sqrt{2}$, A_2, and A_3 are coefficients whose absolute square gives the probability that after the collision the hydrogen and the sodium atoms are in the state indicated by the subscript of the basis function. The basis wave functions $\psi_{H+Na(3P)}$ and $\psi_{H^-+Na^+}$ are used to indicate levels that respectively become H and Na(3P) and H^- and Na^+ in the separated atom limit. In the case of $\psi_{H+Na(3P)}$ and $\psi_{H^-+Na^+}$ we do not explicitly indicate the time and electron spin dependence as is done for $\psi_{{}^3\Sigma}$ and $\psi_{{}^1\Sigma}$. After the collision the probability that the hydrogen atom has $M_1 = -1/2$ and the sodium atom is in the ground level and has $M_2 = 1/2$, so that spin exchange has occurred, is given by $P = |(1-A_1e^{i\phi_{ts}})/2|^2$ where $\phi_{ts} = \int(V_t-V_s)dt/\hbar$.

We first estimate the spin exchange cross section assuming $A_1 = 1$ (i.e. for no reactions that lead to H + Na(3P) or H^- + Na^+). For this situation $P = \sin^2(\phi_{ts}/2)$ where ϕ_{ts} is a function of b and E. The spin exchange cross section is then

$$\sigma = 2\pi\int_0^\infty b\sin^2(\phi_{ts}/2)db \quad (3)$$

We calculate the spin exchange cross section at a given energy by numerically evaluating ϕ_{ts} at a given impact parameter using the H + Na molecular potentials of Olson and Liu [10] assuming a straight line trajectory. We then evaluate the cross section by numerical integration over impact parameters. The potentials are not known for impact parameters less than 0.8Å. We consequently ignore the contribution to σ for impact parameters less than 0.8Å. Our calculations fail at low energies because scattering angles are large enough to invalidate the use of a straight line trajectory, and at high energies because the Born Oppenheimer approximation fails. For H + Na we estimate the calculated spin exchange cross section is satisfactory from about 35 eV up to 5 keV. Fig. 1 shows the calculated spin exchange cross section for H + Na.

We now investigate how the calculated cross sections are altered by other reaction channels. R.E. Olson has sent us the results of calculations he performed [11], giving probabilities, K, that a H atom and a Na atom initially in the $^1\Sigma$ level remain in the $^1\Sigma$ level after a collision. We estimate the effect of other reaction channels on the calculated spin exchange cross sections for a H + Na collision using $A_1 = \sqrt{K}$, to evaluate the probability P. We then obtain the spin exchange cross section at a given energy by integrating over the impact parameters. We find the effect of other reaction channels on the spin exchange cross sections for H incident on Na at energies of 0.5 keV or less reduces the cross sections by less than 15%. At energies of 1 and 2 keV the cross sections are reduced by about 35% and 45% respectively. At 5 keV the spin exchange cross section is reduced by about 25%. The incident H atom can also flip its spin when the Na atom emerges in the 3P level. We have roughly estimated the contribution of this effect on the total probability that a H atom flips its spin when incident on Na at a given impact parameter and energy. From this we estimate the total cross section for the H atom to flip its spin. We find this cross section is only slightly different from the cross section shown in Fig. 1.



(a)

(b)

Fig. 1. Calculated spin exchange cross sections for fast H atoms incident on (a) H, Na and Rb, and (b) Li, K and Cs.

We have also carried out similar calculations of spin exchange cross sections for H incident on H, Li, K, Rb, and Cs and the results are shown in Fig. 1. For these calculations we have used potentials calculated by Sharp (H + H) [12], Stevens et al. (H + Li, H + K and H + Rb) [13], and Jeung et al. (H + Cs) [14]. For H + H the effects of other reaction channels are very small. For H incident on the other alkalis we do not know the effects of other reaction channels but we assume that these effects are relatively small as they are for H + Na.

At a low magnetic field the hyperfine interaction causes the electron spin and the nuclear spin to be coupled to form a total angular momentum F and z component M. The probability in low field that a spin exchange collision takes a H atom initially in state F_1, M_1 and a target atom initially in state F_2, M_2 and leaves them respectively in final states F_1', M_1' and F_2', M_2' can be obtained by decomposing the initial state wave functions into electron spin and nuclear spin basis functions and then calculating the final state wave function in terms of ϕ_{ts}. The probability that the final state is F_1', M_1' and F_2', M_2' must be integrated over all impact parameters to obtain the cross section.

In the optically pumped polarized H^- ion source, H^+ ions are incident with an energy of about 5 keV on an optically pumped electron spin polarized Na vapor target. The H^+ ions pick up a polarized electron in the n = 2 level of the H atom. Radiative decay to the n = 1 level then occurs. In the radiative decay some angular momentum is carried off by the emitted photon so that the electron spin polarization of the fast n = 1 level H atom is less than the electron spin polarization of the Na target. The loss of polarization in the radiative decay depends on the magnetic field at the Na target. Fields of 1 - 2 T are required to prevent significant loss of polarization [3,15]. After the fast n = 1 H atom is produced in the Na target it passes through the remainder of the electron spin polarized Na vapor target where the fast H atoms can make spin exchange collisions which increase the electron spin polarization of the H atoms toward the target polarization. At 5 keV, $\sigma = 1.2 \times 10^{-15}$ cm^2 for H + Na. The effect of spin exchange collisions will be important when $\sigma\pi$ becomes comparable to 0.5 or greater, where π is the Na target thickness in atoms/cm^2. Thus for values of $\pi \geq 4 \times 10^{14}/cm^2$ one expects spin exchange to signficantly increase the polarization of the fast H beam. If one can obtain $\pi \sim 10^{15}/cm^2$ then one may be able to use the optically pumped ion source in a field much less than 1 T and still retain high polarization.

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