PHYSICAL REVIEW
LETTERS

VOLUME 27 | 29 NOVEMBER 1971 | NUMBER 22

Possibility of Producing Spin-Polarized Hydrogen Atoms by Charge-Transfer Collisions with Xe†

J. Macek and R. Shakeshaft
Behlen Laboratory of Physics, University of Nebraska, Lincoln, Nebraska 68508
(Received 7 October 1971)

It is argued that hydrogen atoms formed by charge-transfer reactions with Xe at 15-eV incoming proton energy could be spin polarized. A detailed numerical calculation of the charge-transfer probability and the spin-polarization fraction indicate that a spin polarization as large as 70% may occur while the charge-transfer probability is simultaneously 0.6.

Experiments by Koopman[1] have established that the cross section for the reaction

$$Xe + H^+ \rightarrow Xe^+ + H \quad (1)$$

is very large, of the order of 40×10^{-16} cm^2, for 50-eV protons. Such a large cross section is expected from the Massey criteria[2] for a nearly resonant process. The energy defect of the reaction is 1.5 eV if the Xe^+ is left in its $^2P_{3/2}$ ground state, and is somewhat too large to account for the observed behavior of the cross section. Koopman[1] argues that the polarizability correction suggested by Hasted[3] effectively reduced the energy deficit, thereby accounting for the observed cross section. However, Fleishchman and Young[4] have suggested the alternative interpretation that Xe^+ is left in the excited $^2P_{1/2}$ state for which the energy defect is 0.17 eV without invoking the polarizability correction. Since the observed cross section indicates that charge transfer must occur for impact parameters as large as 7 a.u., and since here the polarizability potential energy is small compared to 1.5 eV, it seems that this latter interpretation is more reasonable. In this note we point out that, with this latter interpretation, the scattered hydrogen atoms may be spin polarized. We have checked the interpretation by a detailed numerical calculation, have found it substantially correct, and have evaluated the degree of spin polarization. For 15-eV protons we find a spin polarization as large as 70%. To our knowledge this represents the first indication that spin-polarized hydrogen atoms may be produced by charge-transfer collisions.

That Reaction (1) may produce spin-polarized protons can be visualized by a simple geometrical construction.[5] The internal electronic angular momentum of the initial $Xe + H^+$ system is zero while the final angular momentum of the $Xe^+(^2P_{1/2}) + H(^2S_{1/2})$ system is zero or unity on the basis of vector coupling rules. However, invariance of the system under reflections in the plane defined by the momenta of the incoming and outgoing particles rules out the $J=0$ state. This selection rule is important for our construction and is obtained by representing the reflection operator Y in the form[6]

$$Y = \exp(-i\pi J_y)P, \quad (2)$$

where the x-z plane represents the scattering plane with the z axis oriented parallel to the momenta of the incoming H^+, and P is the internal parity operator. For $J=0$ states the eigenvalues of Y equal the eigenvalues of P, but the eigenvalue of P changes sign in the charge-transfer collision. Therefore, a $J=0$ final state cannot be formed; only the $J=1$ final states can. Because such states transform as vectors, and because of

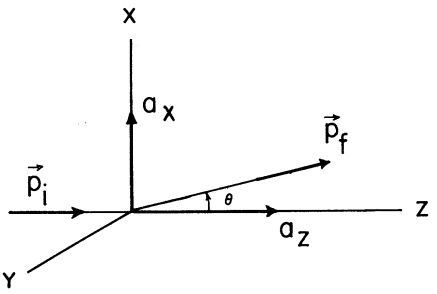

FIG. 1. Diagram illustrating the coordinate system and its relation to the initial and final relative momentum vectors. The two possible charge-transfer states of $Xe^+(^2P_{1/2})+H$ are represented by vectors parallel to the x and z axes. The length of the vectors represent the amplitudes a_x and a_z for forming the two states.

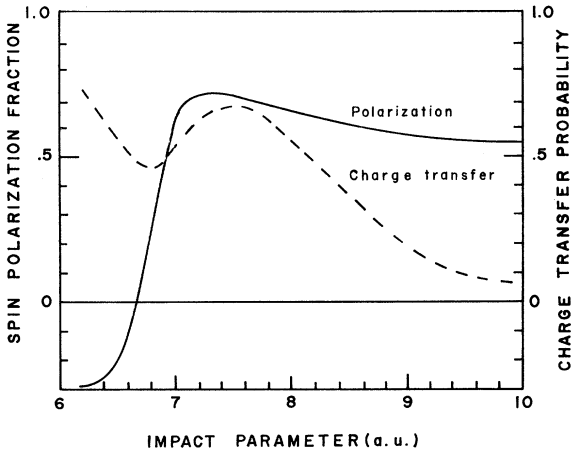

FIG. 2. Calculated spin-polarization fraction and charge-transfer probabilities. Positive polarization corresponds to hydrogen-atom spin aligned along the vector $\vec{p}_i \times \vec{p}_f$. The incident proton energy is 15 eV.

reflection invariance, they may be represented by only two vectors, one oriented along the z axis and one along the x axis (Fig. 1). The lengths of the vectors correspond to the magnitudes of the amplitudes a_z and a_x for exciting the two states. When a_z and a_x are equal and out of phase by 90°, the state formed is represented by a vector rotating about the y axis, i.e., the coherent superposition of the two states formed in the collision is represented by the $M=+1$ (or -1) component of the spherical basis vectors with the y axis taken as the axis of quantization.[7] If only one of these states, M = 1, is populated, then both the spin of the $H(^2S_{1/2})$ and the internal angular momentum of the $Xe^+(^2P_{1/2})$ states are aligned corresponding to 100% spin polarization of the hydrogen atom. For arbitrary values of a_z and a_x the fraction of hydrogen atoms spin polarized along the y axis is easily found by resolving the vectors into spherical components with the y axis as the quantization axis. We find

$$P_y = -\frac{2|a_x a_z| \sin\Delta}{|a_x|^2 + |a_z|^2}, \tag{3}$$

where P_y is the fraction of hydrogen atoms spin polarized along the y axis, and where Δ is the phase difference between a_z and a_x. For $\Delta \neq 0$, $a_z \neq 0$, and $a_x \neq 0$, the polarization is nonzero, and thus the possibility of spin polarization is indicated independent of a detailed calculation. We have made such a calculation, however, in order to determine the range of physical parameters which favor such processes.

We have formulated an atomic-state eigenfunction expansion applicable to atoms whose states are eigenstates of electronic angular momentum only rather than both spin and orbital angular momentum. This formalism closely parallels Wilets and Gallaher's[8] treatment of $H^+ + H$ collisions, and will be reported elsewhere.[9] To apply it to the present problem we have used Herman-Skillman[10] potentials and outer-shell $5p$ wave functions to describe Xe, $Xe^+(^2P_{3/2,1/2})$, and the interaction of the hydrogen-atom electron with Xe^+. Since the energy defect governs the behavior of the cross section at low energies and large impact parameters, we have used the experimental energies rather than the model energies. By this means the spin-orbit coupling is introduced into the model in such a way that it operates to populate preferentially the $^2P_{1/2}$ state exactly as it does in the physical reaction, namely, by splitting the $^2P_{3/2,1/2}$ energies of Xe^+. The model is reliable as long as the hydrogen-atom wave function does not penetrate significantly into the Xe^+ core. Since the calculations reported here are restricted to impact parameters greater than 6 a.u., this condition is satisfied. Furthermore, we find that contributions from charge transfer leaving Xe^+ in the $^2P_{3/2}$ state are less than 10% for impact parameters of the order of 6 a.u. and decrease rapidly for increasing impact parameter; therefore, such contributions are neglected in the calculations used here.

Figure 2 shows the calculated spin polarization for 15-eV protons incident upon Xe, with the corresponding charge-transfer probabilities.

The most favorable combination of polarization and charge-transfer probabilities occurs at an impact parameter of 7.2 a.u. Here P_y equals 72%, while 60% of the scattered particles are

hydrogen atoms. To completely specify the conditions for which such polarization may be observed, it is necessary to relate the amplitudes which are functions of impact parameter to amplitudes which are functions of scattering angle. Indeed, the amplitudes in Eq. (3) are functions of scattering angle. However, we have supposed that the use of amplitudes which are functions of impact parameter will give an adequate estimate of the expected polarization. Rigorous expressions involving integrals over Bessel functions relating the two alternative sets of amplitudes have been given in the literature.[11] The argument of the integral oscillates considerably, and thus an approximate correspondence of impact parameter b with scattering angle can be obtained using a stationary-phase approximation to evaluate the integrals.[12] In this way we estimate that $b = 7.2$ a.u. corresponds to a scattering angle of 2.6°, while $b = 6.6$ a.u. corresponds to 3.4° and $b = 8.0$ a.u. corresponds to 2°.

†Work partially supported by the National Science Foundation.

[1]D. W. Koopman, Phys. Rev. 154, 79 (1967).

[2]H. S. W Massey and E. H. S. Burhop, *Electronic and Ionic Impact Phenomena* (Oxford U. Press, New York, 1952), p. 50.

[3]J. B. Hasted and A. R. Lee, Proc. Phys. Soc. (London) 79, 702 (1962).

[4]H. H. Fleischmann and R. A. Young, Phys. Rev. Lett. 19, 941 (1967).

[5]A similar construction was employed by one of the present authors to discuss the polarization of optical radiation following collision excitation. See J. H. Macek and D. H. Jaecks, Phys. Rev. A (to be published).

[6]M. Goldberger and K. Watson, *Collision Theory* (Wiley, New York, 1964), p. 885.

[7]M. E. Rose, *Elementary Theory of Angular Momentum* (Wiley, New York, 1957), p. 103.

[8]L. Wilets and D. E. Gallaher, Phys. Rev. 147, 13 (1966).

[9]R. Shakeshaft and J. Macek, to be published. See also the "Seventh International Conference on the Physics of Electronic and Atomic Collisions. Abstracts of Papers," edited by J. B. Hasted (North-Holland, Amsterdam, to be published).

[10]F. Herman and S. Skillman, *Atomic Structure Calculations* (Prentice-Hall, Englewood Cliffs, N. J.).

[11]L. Wilets and S. J. Wallace, Phys. Rev. 169, 84 (1968).

[12]N. F. Mott and H. S. W. Massey, *Theory of Atomic Collisions* (Oxford U. Press, London, 1965), p. 100.

Penning Ionization in a He-Cd dc Discharge

W. T. Silfvast

Bell Telephone Laboratories, Holmdel, New Jersey 07733

(Received 12 January 1971)

Penning ionization is shown to be the dominant ionization mechanism in a low-current He-Cd dc discharge under certain conditions. Properties of a discharge of this type are discussed.

Penning ionization was suggested by this author as being responsible for the excitation of the Cd^+ laser levels in a He-Cd dc discharge.[1] This Letter reports some results of studies made in low-current He-Cd dc discharges under conditions where the Penning ionization process is optimized. Experimental evidence is presented which indicates that, at certain partial pressures of Cd vapor, Penning collisions are the dominant source of ionization in the discharge and virtually the only source of excitation of excited Cd^+ levels.

In a He-Cd dc discharge, from the consideration of the densities of various energy carrying species and estimates of their relative excitation cross sections, it is expected that the processes resulting in significant excitation of the Cd^+ levels would be electron impact ionization, charge transfer from He^+ and He_2^+, and Penning ionization by He metastables. Schearer and Padovani[2] have demonstrated the dominance of the Penning reaction in a pulsed He-Cd afterglow where the only significant energetic species are He^+ and He $2s\,^3S$ metastables. They also measured the total Penning cross section (4.5×10^{-15} cm^2) from the ^3S metastable to all of the energetically accessible Cd^+ levels[2]; however, cross sections to specific levels are not accurately known. Also, Penning cross sections from the He $2s\,^1S$ metastable and charge-transfer and electron-excitation cross sections to most of the excited Cd^+ levels are not known.

We will consider the effect of Penning collisions on the $5s^2\,^2D$, $6s\,^2S$, and $5d^2\,^2D$ levels of Cd^+. These levels have no cascade excitation