J. Phys. B: At. Mol. Opt. Phys. **22** (1989) 2387-2392. Printed in the UK

Total electron scattering cross sections for molecular hydrogen at low electron energies

K P Subramanian and Vijay Kumar

Physical Research Laboratory, Navrangpura, Ahmedabad-380009, India

Received 14 December 1988, in final form 1 March 1989

Abstract. Absolute total electron scattering cross sections for molecular hydrogen have been measured at low electron energies using a photoelectron source. The measurements have been carried out at 25 electron energies varying from 0.2 to 10 eV with an accuracy of ±2.7%. The cross sections obtained in the present experiment have been compared with other recent measurements and theoretical computations.

Electron-atom and electron-molecule collision processes are known to play an important role in various areas, with practical applications in the fields of gaseous lasers, planetary atmospheres and interstellar clouds, gaseous dielectrics and magneto-hydrodynamic plasmas. These fields require accurate knowledge of electron-atom and electron-molecule total scattering cross sections at low electron energies. As a result, interest in both experimental as well as theoretical aspects of the subject has grown enormously in the last decade.

Hydrogen, being the simplest neutral molecule, has been extensively studied theoretically (Hara 1969, Morrison and Saha 1986, Morrison *et al* 1987 and many other researchers referred to in the review article by Lane 1980). A large number of measurements have also been made to obtain absolute total $e^- - H_2$ scattering cross sections at low electron energies. These include measurements made by Golden *et al* (1966), Dalba *et al* (1980), Ferch *et al* (1980), Hoffman *et al* (1982), Deuring *et al* (1983) and Jones (1985). The agreement between measured and theoretically computed values of cross sections appears to be only marginal indicating that more measurements in this direction are needed, possibly using new techniques.

This paper presents the measurement of absolute total electron scattering cross sections for molecular hydrogen at 25 energy points in the electron energy region from 0.2 to 10 eV. In this experiment, the electrons produced conventionally from guns have been replaced by photoelectrons produced by the interaction of monochromatic VUV photons with source gases such as noble atoms as well as with molecular hydrogen itself. Previously, absolute electron scattering cross sections for helium, neon, argon, krypton and xenon have been reported by the authors in a similar electron energy range (from 0.7 to 10 eV) using the same technique (Kumar *et al* 1987, Subramanian and Kumar 1987). The present paper is an attempt to take up the electron scattering cross section measurement of molecules at low electron energies.

A detailed description of the experimental set up used for this study, method for analysis of the data and error analysis has been given in two previous publications (Kumar *et al* 1987, Subramanian and Kumar 1987). A brief description is given here for the sake of completeness. Photoelectrons are produced by the interaction of

0953-4075/89/152387+06$02.50

monochromatic VUV photons with a source gas such as argon, krypton, xenon or molecular hydrogen itself. With argon, krypton or xenon, electrons of two energies corresponding to the $^2P_{1/2}$ and $^2P_{3/2}$ states of the ions are produced. With molecular hydrogen, photoelectrons of different energies corresponding to vibrational levels from $v \geqslant 0$ of the $X\,^2\Sigma_g^+$ state of the molecular ions are produced. With photons of a single wavelength and using one source gas at a time, electrons with different energies would be accessible. Using different combinations of photons of three different wavelengths (He I, 58.4 nm, Ne I, 73.6 and 74.4 nm) and four different source gases, and neglecting the energy points where the statistics for the photoelectron intensity was poor, it was possible to measure scattering cross sections at 25 electron energies. These energies along with the photon wavelengths, source gas and photoion state produced are given in table 1.

The photoelectrons produced in the ionising region were allowed to be scattered by the target gas. Without any target gas, the amplitudes of the photoelectron peaks produced by the source gas were monitored at a fixed but low source gas pressure in the ionisation region. The target gas was then introduced and if the source gas and the target gas were not the same, the amplitudes of the photoelectron peaks would decrease with increasing target-gas pressure. This decrease was attributed to electron scattering by the target-gas species whose number density increases with increasing

Table 1. Total electron scattering cross sections for molecular hydrogen at various electron energies. Also given are the photon wavelength, the source gas and the photoion state for the corresponding electron energy.

Photon wavelength (Å)	Source gas	Photoion state	Electron energy (eV)	Scattering cross section (Å^2)
736	Hydrogen	$v=5$, $X\,^2\Sigma_g^+$	0.21	11.47
736	Hydrogen	$v=4$, $X\,^2\Sigma_g^+$	0.42	11.28
736	Hydrogen	$v=3$, $X\,^2\Sigma_g^+$	0.64	11.54
744	Argon	$^2P_{1/2}$	0.73	12.39
736	Hydrogen	$v=2$, $X\,^2\Sigma_g^+$	0.88	12.66
736	Argon	$^2P_{3/2}$	1.09	13.67
736	Hydrogen	$v=1$, $X\,^2\Sigma_g^+$	1.14	13.64
744	Krypton	$^2P_{1/2}$	2.00	15.59
736	Krypton	$^2P_{1/2}$	2.18	16.03
744	Krypton	$^2P_{3/2}$	2.66	16.18
736	Krypton	$^2P_{3/2}$	2.85	16.46
744	Xenon	$^2P_{1/2}$	3.23	16.30
736	Xenon	$^2P_{1/2}$	3.41	16.34
584	Hydrogen	$v=6$, $X\,^2\Sigma_g^+$	4.38	15.65
584	Hydrogen	$v=5$, $X\,^2\Sigma_g^+$	4.58	15.75
744	Xenon	$^2P_{3/2}$	4.59	15.60
736	Xenon	$^2P_{3/2}$	4.77	15.22
584	Hydrogen	$v=4$, $X\,^2\Sigma_g^+$	4.78	15.60
584	Hydrogen	$v=3$, $X\,^2\Sigma_g^+$	5.01	15.28
584	Hydrogen	$v=2$, $X\,^2\Sigma_g^+$	5.24	14.85
584	Hydrogen	$v=1$, $X\,^2\Sigma_g^+$	5.50	14.57
584	Krypton	$^2P_{1/2}$	6.55	13.67
584	Krypton	$^2P_{3/2}$	7.22	13.05
584	Xenon	$^2P_{1/2}$	7.78	12.22
584	Xenon	$^2P_{3/2}$	9.14	11.23

pressure. When the source and target gas were the same, as in the case of molecular hydrogen itself, the amplitudes of the photoelectron peaks would first increase with increasing source/target gas pressure but would start decreasing with subsequent increase in pressure. At low gas pressures, the photoelectron production rate dominates over the electron-molecule scattering but, at higher pressures, the contribution due to electron scattering becomes significantly larger.

The microwave discharge light source for producing resonant emission lines of helium and neon, the beam splitter for monitoring any change in the intensity of the incident photon beam, the ionisation and scattering regions, the cylindrical mirror analyser, the electron detector, channeltron and data acquisition system have been described in detail previously (Kumar *et al* 1987, Subramanian and Kumar 1987). The pumping systems and additional fast pumps for differential pumping of the various regions including the ionisation region and some regions of the cylindrical mirror analyser and electron detector have also been discussed there. The details of absolute pressure measurement using an MKS capacitance manometer and the performance of the photoelectron spectrometer have been given in one of our previous publications (Kumar *et al* 1987).

The electron scattering cross sections for molecular hydrogen were measured using the method described previously. When source and target species are different, the electron scattering cross sections, σ, can be evaluated by using the following equation:

$$\ln\left(\frac{I_{e2}}{I_{e1}}\frac{I_{\lambda 01}}{I_{\lambda 02}}\right)=\frac{P_1-P_2}{760}[n_0\sigma x+k(al_1+l_2)] \tag{1}$$

where I_{e1} and I_{e2} are the amplitudes of the photoelectron peaks at two different gas pressures P_1 and P_2, $I_{\lambda 01}$ and $I_{\lambda 02}$ are the incident photon intensities monitored by the beam splitter at the two pressures, l_1 is the distance from the centre of the beam splitter to the circular aperture covering the ionisation region, l_2 is the distance from the same aperture to the actual ionisation region defined geometrically by the different slits in the accelerating region and cylindrical mirror analyser, x is the scattering pathlength, a is the ratio of the pressures of the target gas outside and inside the ionising region while k is the photoabsorption coefficient of the target gas at a particular photon wavelength. The total photoabsorption cross sections at the three incident photon wavelengths have been taken from Lee *et al* (1976). The ratio of $I_{\lambda 01}$ to $I_{\lambda 02}$ could be determined from the beam splitter.

When source and target-gas species are the same, the electron scattering cross section could be evaluated by an equation given below:

$$\ln\left(\frac{I_{e2}}{I_{e1}}\frac{I_{\lambda 01}}{I_{\lambda 02}}\frac{P_1}{P_2}\right)=\frac{P_1-P_2}{760}[n_0\sigma x+k(al_1+l_2)]. \tag{2}$$

All errors in the measurement of electron scattering cross sections have been discussed in detail previously (Kumar *et al* 1987). In the present experiment, the most probable error was estimated to be ±2.7%.

The electron scattering cross sections for molecular hydrogen were measured using equations (1) and (2) respectively in the two cases described above. In both these equations, all the parameters I_{e1}, I_{e2}, $I_{\lambda 01}$, $I_{\lambda 02}$, P_1 and P_2 could be determined experimentally and cross sections could be calculated.

The total electron scattering cross sections for molecular hydrogen as measured in the present experiment are shown in figure 1 for electron energies ranging from 0.2 to 10 eV. Also, the error bars are shown in the figure at three energies only. The lowest

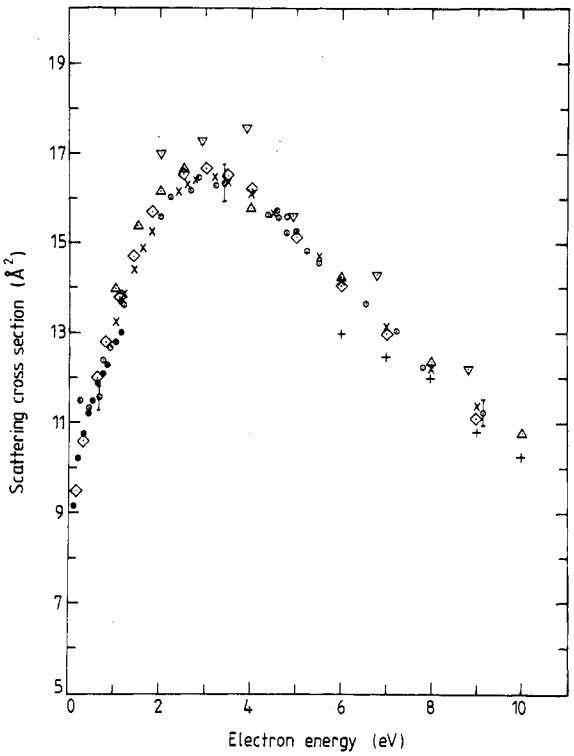

Figure 1. Total electron scattering cross sections for molecular hydrogen as a function of incident electron energy from 0.2 to 10 eV obtained by various researchers. △, Dalba *et al* (1980); ●, Ferch *et al* (1980); ▽, Hoffmann *et al* (1982); +, Deuring *et al* (1983); ×, Jones (1985); ◇, Morrison *et al* (1987); ⊙, present results.

energy was 0.21 eV and it was not possible to go to energies below this value because of constraints on the photon beam wavelengths and the type of source gases available to us. Starting from this energy, there was a steep rise in cross sections with a broad structureless maximum around 2.85 eV and above this energy the cross sections decreased steadily with increasing electron energy. This broad maximum observed by other researchers previously was attributed to the formation of a shape resonance (Bardsley *et al* 1966, Ehrhardt *et al* 1968). The temporary state involved is the $^2\Sigma_u^+$ of the H_2^- ion having short lifetime.

A comparison of the cross sections measured in the present experiment has been made with a few prior experimental results and some theoretical calculations. The cross sections measured by Dalba *et al* (1980), Ferch *et al* (1980), Hoffman *et al* (1982), Deuring *et al* (1983) and Jones (1985) and calculated by Morrison *et al* (1987) have been shown in figure 1 along with the results obtained in the present experiment. Some of the work reported previously was contributed by Bruche (1927), Ramsauer and Kollath (1930) (using the Ramsauer type of transmission technique) and by Golden *et al* (1966) using a modified Ramsauer method. Similar contributions giving computed cross sections were reported by Wilkins and Taylor (1967) using a Hartree-Fock approach, Hara (1969) using a two-centre calculation including polarisation and by Henry and Lane (1969) using a close-coupling computational method including polarisation. All these results were in good agreement in regard to the general shape of the

total cross section curve but, quantitatively, there was only a marginal agreement between them.

The cross sections measured by Dalba *et al* (1980), shown in figure 1 along with the results given by the authors, were obtained using a linear transmission technique with an electrostatic energy analyser. Their experiment covered an electron energy range from 0.2 to 100 eV with an overall error ranging from ±7% at the lowest electron energy to ±1.7% at 15 eV. Our results are in reasonably good agreement with those given by Dalba *et al* within the stipulated experimental error. In comparison, the cross sections reported by Hoffman *et al* (1982) are consistently larger than the present measurements at all energies except one. At 4.9 eV the cross section given by Hoffman *et al* is in good agreement with that reported in the present experiment but at all other energies the values of cross sections are higher by about 6 to 9%. It may be pointed out here that the measurements by Hoffman *et al* were carried out using a beam transmission technique at energies 2 to 500 eV with an accuracy of ±5%.

Deuring *et al* (1983) using a linear transmission technique reported cross sections at only five energies between 6 and 10 eV with a total systematic error of ±5%. Their values are, in general, smaller than given in the present experiment. A time-of-flight electron transmission spectrometer was employed by Jones (1985) to measure absolute cross sections at electron energies ranging from 1 to 50 eV. The accuracy reported in his experiment was better than ±2.6% below 10 eV. There seems to be an excellent agreement of the cross section data reported by Jones (1985) and by the authors in the present work.

The cross sections measured in the present experiment have been compared with theoretically computed values given by Morrison *et al* (1987) and Hara (1969). The total integrated cross sections calculated by Morrison *et al* take account of vibrational and rotational excitations of the target. Adiabatic nuclei calculations including exact static exchange with polarisation were used for the elastic contribution and a full rovibrational laboratory-frame close-coupling calculation with exchange and polarisation was employed to obtain the inelastic contribution. Their results are in excellent agreement with the present measurements at all energies except the lowest. Hara (1969) calculated the integral elastic cross sections using a fixed-nuclei adiabatic-exchange approximation with polarisation and exchange included. Hara's results do not include the vibrationally inelastic contribution to the total cross section. As a result, his values of cross sections are consistently lower at all energies. For this reason, the cross sections computed by Morrison *et al* have only been included in figure 1.

At very low electron energies below 0.4 eV, there seems to be some disagreement in the shape of the cross section curve. The measurements by Ferch *et al* (1980) made with an electron time-of-flight spectrometer in the energy range from 0.02 to 2 eV and cross sections computed by Morrison *et al* (1987) showed a steep decrease at low electron energies. The zero-energy cross sections when extrapolated would have a value less than 8 $Å^2$. This does not seem to be the case in the present measurement. Though there is good agreement in the values of the cross sections up to 0.42 eV, the cross section at 0.21 eV does not decrease in the same way as in the other two cases, but has almost the same value as at two previous energies. This fact has been ascertained by repeating the measurements at low energies a few times. In our experiment it is not possible to have more energy points at electron energies below 0.21 eV because of constraints due to the light source used in the experiment. It is, therefore, suggested that cross section measurements at electron energies below 0.4 eV should be carried out again by different research groups using different techniques.

The values of the cross sections for molecular hydrogen as measured in the present experiment are given in table 1.

References

Bardsley J N, Herzenberg A and Mandl F 1966 *Proc. Phys. Soc.* **89** 321-40
Bruche E 1927 *Ann. Phys., Lpz.* **82** 912-46
Dalba G, Fornasini P, Lazzizzera I, Ranieri G and Zecca A 1980 *J. Phys. B: At. Mol. Phys.* **13** 2839-48
Deuring A, Floeder K, Fromme D, Raith W, Schwab A, Sinapius G, Zitzewitz P W and Krug J 1983 *J. Phys. B: At. Mol. Phys.* **16** 1633-56
Ehrhardt H, Langhans L, Linder F and Taylor H S 1968 *Phys. Rev.* **173** 222-30
Ferch J, Raith W and Schroder K 1980 *J. Phys. B: At. Mol. Phys.* **13** 1481-90
Golden D E, Bandel H W and Salerno J A 1966 *Phys. Rev.* **146** 40-2
Hara S 1969 *J. Phys. Soc. Japan* **27** 1009-19
Henry R J W and Lane N F 1969 *Phys. Rev.* **183** 221-31
Hoffman K R, Dababneh M S, Hsieh Y F, Kauppila W E, Pol V, Smart J H and Stein T S 1982 *Phys. Rev.* A **25** 1393-403
Jones R K 1985 *Phys. Rev.* A **31** 2898-904
Kumar V, Krishnakumar E and Subramanian K P 1987 *J. Phys. B: At. Mol. Phys.* **20** 2899-910
Lane N F 1980 *Rev. Mod. Phys.* **52** 29-119
Lee L C, Carlson R W and Judge D L 1976 *J. Quant. Spectrosc. Radiat. Transfer* **16** 873-7
Morrison M A, Crompton R W, Saha B C and Petrovic Z Lj 1987 *Aust. J. Phys.* **40** 239-81
Morrison M A and Saha B C 1986 *Phys. Rev.* A **34** 2786-97
Ramsauer C and Kollath R 1930 *Ann. Phys., Lpz.* **4** 91-108
Subramanian K P and Kumar V 1987 *J. Phys. B: At. Mol. Phys.* **20** 5505-15
Wilkins R L and Taylor H S 1967 *J. Chem. Phys.* **47** 3532-9