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Elastic scattering and rovibrational excitation of H_2 by low-energy electrons

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Abstract. We report differential and integral cross sections for elastic scattering and rovibrational ($v = 0 \rightarrow 1$) excitation of H_2 by electrons at seven energies in the range 1-5 eV. The measurements were conducted on a fine energy grid in an attempt to resolve an impasse that had arisen between theory and 'swarm' derived cross sections and to enable a detailed comparison to be made with the best available theoretical calculations.

1. Introduction

Just as an understanding of the dynamics of electron scattering from atomic hydrogen is central to the study of atomic systems, the interaction of low-energy electrons with molecular hydrogen is the most fundamental electron-molecule collision process one can study. It is thus somewhat surprising that there exist only a few measurements of absolute elastic and rovibrational excitation ($v = 0 \rightarrow 1$) cross sections at energies below 5 eV, and even fewer detailed theoretical calculations for these processes.

A comprehensive discussion of the earlier measurements and the current status of experiment and theory for low-energy electron-H_2 scattering has been given in a preliminary report (Brunger *et al* 1990) of some aspects of this work and so here we simply reference the earlier work for completeness. Differential and integral elastic and rovibrational scattering measurements have been carried out previously by Ehrhardt *et al* (1968), Linder and Schmidt (1971) and Nishimura *et al* (1985) whilst measurements solely for elastic scattering have been reported by Shyn and Sharp (1981) and Furst *et al* (1984). There has been a number of swarm studies of electrons in molecular hydrogen. The most recent, in which the momentum transfer cross section for elastic scattering and total cross sections for rotational and rovibrational excitation have been derived, is that of England *et al* (1988). The theoretical studies have been largely restricted to a few groups (e.g. Henry and Lane 1969, Morrison *et al* 1984) and of these the most extensive effort has clearly been made by Morrison and his co-workers. A detailed summary of these calculations has been given by Morrison *et al* (1987).

The level of quantitative agreement between the experiments themselves and between theory and experiment, would appear to be fair for elastic scattering and rotational excitation (Morrison *et al* 1987). However, the situation for rovibrational excitation is far from satisfactory as, from the earliest measurements, there has been a serious discrepancy in the near-threshold behaviour of this integral cross section as derived from swarm experiments (Compton *et al* 1970, England *et al* 1988) and that measured in beam studies (Ehrhardt *et al* 1968, Linder and Schmidt 1971). Indeed it

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was this disagreement that prompted the rigorous theoretical programme embarked upon by Morrison and his co-workers. These calculations (Morrison *et al* 1987) resulted in a rovibrational excitation cross section which was in good agreement with the beam cross sections at energies greater than about 0.3 eV above threshold (0.52 eV) but not with the swarm cross section. Notwithstanding this, Morrison *et al* (1987) expressed some doubts as to the accuracy of the earlier beam measurements (Ehrhardt *et al* 1968, Linder and Schmidt 1971) on the basis that the primary aim of these earlier investigations was the study of resonance effects in electron-H_2 scattering and not the derivation of absolute scattering cross sections. Hence, one of the principal motivations of the present study was to provide a significant body of both differential and integral cross sections against which the most recent calculations (Snitchler *et al* 1990) could be compared and, in the process, hopefully shed some light on the impasse that currently exists between the swarm derived and theoretically calculated rovibrational integral cross section.

In section 2 we describe the experimental apparatus and the techniques employed in the current measurements. Section 3 contains the present results and a discussion of their implications, while in section 4 we provide some concluding remarks.

2. Experimental apparatus and technique

The present measurements have been carried out with the aid of a high resolution electron monochromator. A description of the apparatus, which is schematically presented in figure 1, and its principles of operation, was given previously by Brunger *et al* (1990). Briefly, however, a beam of H_2 effusing from a multichannel capillary array of active diameter 1 mm is crossed with a beam of monoenergetic electrons of desired

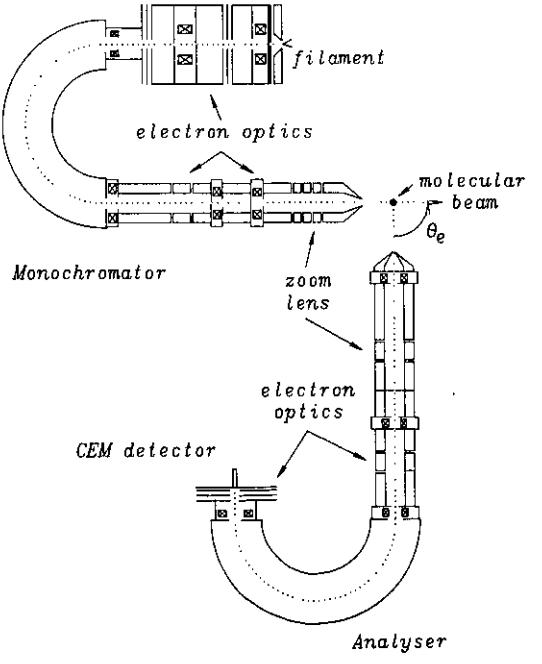

Figure 1. Schematic diagram of the electron monochromator.

energy E_0. Vibrationally elastic (henceforth referred to as 'elastic') and inelastically scattered electrons at a particular scattering angle (θ) are energy analysed and detected. The energy resolution in the present measurements was detuned to typically 90 meV (FWHM). This was sufficient to separate the $v = 0 \rightarrow 1$ rovibrational transition and the elastic excitation from each other, but insufficient to resolve any rotational structure. A typical energy-loss spectrum, shown in figure 2, clearly demonstrates this point.

Care was taken to reduce stray electric fields to an insignificant level and to minimize the ambient magnetic field at the interaction volume which was located at the centre of a set of three pairs of mutually orthogonal rectangular Helmholtz coils. These coils together with magnetic shielding inside the vacuum manifold, enabled the ambient magnetic field to be reduced to less than 10^{-7} T. Proper alignment of the crossed electron and molecular beams and a generous viewing angle for the analyser ensured that no vignetting of this interaction volume occurred in the present system. This was confirmed by the excellent agreement obtained when we measured elastic angular distributions for helium, at each E_0 studied, and compared them to the results of the *ab initio* calculation of Nesbet (1978).

Conditions under which the spatial distribution of the molecular beam was well defined (Brunger *et al* 1990) and the electron beam was stable were maintained throughout. The true zero scattering angle was determined as that about which the intensity of elastically scattered electrons and/or those producing $v = 0$–1 rovibrational excitation was symmetric. The estimated error in this determination is ±1°. The energy scale was calibrated against the well known 2^2S resonance in helium at 19.367 eV and is estimated to be accurate to better than 50 meV.

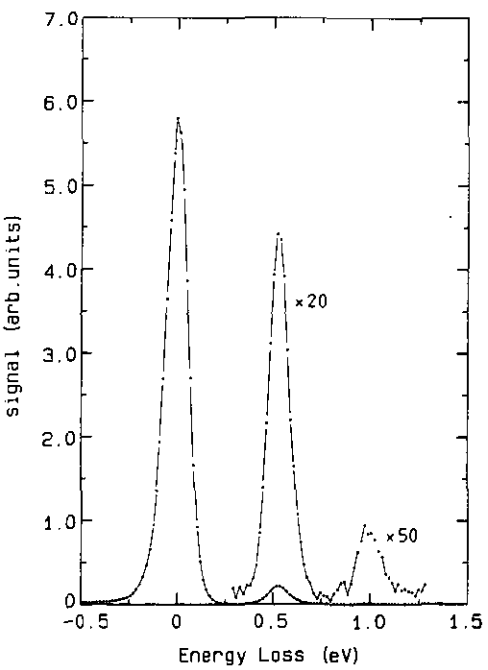

Figure 2. Energy loss spectrum for molecular hydrogen at an incident energy of 3.0 eV and a scattering angle of 50°. The upper spectrum of the $v = 0$–1 feature has been enhanced by a factor of 20, while the upper spectrum of the $v = 0$–2 feature has been enhanced by a factor of 50.

2.1. Normalization

2.1.1. The relative flow technique: elastic scattering. This technique compares the intensity of elastically scattered electrons from two target species, the cross section for one of which is 'known', whilst keeping as many experimental parameters as possible constant during the measurement. In the present case the known cross section is that for helium via Nesbet's calculation. The differential cross section for elastic scattering from H_2 is obtained from the relationship (Srivastava *et al* 1975, Khakoo and Trajmar 1986, Nickel *et al* 1989)

$$\frac{d\sigma}{d\Omega}(\theta)_{H_2} = \frac{I_{He}}{I_{H_2}} \frac{N_e(\theta)_{H_2}}{N_e(\theta)_{He}} \left(\frac{M_{He}}{M_{H_2}}\right)^{1/2} \frac{F_{He}}{F_{H_2}} \frac{d\sigma}{d\Omega}(\theta)_{He} \tag{1}$$

where $N_e(\theta)$ are the scattered electron count rates, M the molecular weight, F the flow rates of the gas through the capillary array and I the electron beam current.

To ensure the establishment of proper flow conditions (Brunger *et al* 1990) one could, in principle, monitor the relative number density directly behind the capillary array or the relative flow rate through the capillary array. However, there are severe practical problems associated with the measurement of pressure and temperature right at the entrance of the capillary tubes, or with the measurement of very low flow rates, so neither of the aforementioned methods are convenient or reliable (Nickel *et al* 1989). A more practical method is to calibrate the relative flow rates for both gases in terms of the respective capillary driving pressures which are readily measured in our case by a capacitance manometer.

In a separate series of experiments we have measured the respective relative flow rates of helium and molecular hydrogen as a function of their capillary driving pressures. The technique employed in these measurements is very similar to that comprehensively described in Khakoo and Trajmar (1986) and so, in the interests of brevity, we do not go into detail here. The results of the present calibration for H_2 and He are given in figure 3, the driving pressures in our case being measured by an MKS Baratron capacitance manometer. In addition the driving pressures are carefully adjusted for each scattering measurement so that the mean free path for each gas at the entrance to the capillary array is identical. Under these circumstances equation (1) can be rewritten into the, experimentally, more amenable form (Srivastava *et al* 1975)

$$\frac{d\sigma}{d\Omega}(\theta)_{H_2} = \frac{I_{He}}{I_{H_2}} \frac{N_e(\theta)_{H_2}}{N_e(\theta)_{He}} \frac{P_{He}}{P_{H_2}} \frac{d\sigma}{d\Omega}(\theta)_{He} \tag{2}$$

where P is the capillary driving pressure for each gas. Equation (2) thus allows us to place our relative angular distribution for elastic e–H_2 scattering on an absolute scale.

2.1.2. Rovibrational excitation. The angular distribution for rovibrational excitation was placed on an absolute scale by measuring, at various scattering angles, the ratio of the scattered intensity for $v = 0 \rightarrow 1$ excitation to that for elastic scattering. Provided the criteria we discuss below are met, this ratio is equivalent to the ratio for the respective differential cross sections, at these scattering angles. Thus, from the previously determined elastic differential cross sections, the differential cross sections for rovibrational excitation could also be placed on an absolute scale. In principle, normalization can be achieved from a measurement of the ratio at a single scattering angle. In practice, the ratios were measured at a number of forward, middle and backward scattering angles. The absolute differential cross sections derived from each of these ratio determinations were found to be consistent.

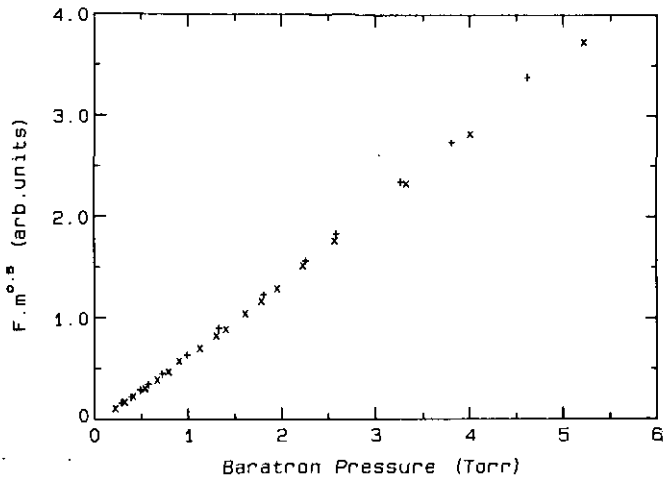

Figure 3. Calibration of the relative flow rates of H_2 (+) and He (×) in terms of the respective capillary driving pressures.

For such an experiment it is important to know the transmission of the scattered electron analyser as a function of energy. This is especially true when the energies of the scattered electrons involved in the measurement are small. For example, for the present measurements at an incident energy of 1.0 eV, the outgoing electrons of interest have energies centred about 1.0 and 0.48 eV. In such a case, the voltage ratio across the analyser zoom lens varies by more than a factor of two and, unless particular care is taken with the operations of this lens, the analyser optics can become severely chromatic. To alleviate such problems in the present ratio measurements, the relative transmission of the analyser over the energy loss range of interest has been optimized by changing the mid-element potential of the analyser zoom lens synchronously with the energy loss voltage. Physically this corresponds to maintaining the image-distance and magnification of the zoom lens constant, irrespective of the energy loss. Great care was taken to ensure this criterion was met for the present experiments and we are confident that this care has indeed enabled us to optimize the analyser transmission to a high level of accuracy.

The technique we employed to calibrate the transmission of the analyser was first explored by Pichou *et al* (1976) and was discussed in detail previously by Brunger *et al.* Briefly, it relies on the fact that up to some value of the incident electron beam energy E_{max} above the ionization threshold, the yield of ionizing (scattered plus ejected) electrons from helium, following near-threshold ionization, is both isotropic and independent of energy. Thus any energy dependence of the yield as recorded by the detector directly reflects the non-uniform transmission of the analyser.

Brunger *et al* (1990) carried out such a measurement and found that for an incident electron energy of 30.08 eV (i.e. 5.5 eV above threshold) the yield of ionizing electrons from 120 meV to 5.5 eV, which encompasses the residual energy range pertaining to the present experiments, was essentially energy independent. However, there is some uncertainty in the range of validity of the Wannier theory (i.e. in E_{max}) with some measurements (Schubert *et al* 1981, Keenan *et al* 1982, Sohn *et al* 1983) indicating that for our present value of $E_{max} = 30.58$ eV the Wannier theory is still valid, whilst others (Hammand *et al* 1985) show that there are departures from this theory at excess

energies as low as 0.075 eV. More recently Nickel *et al* (1989) have asserted that the Wannier law should be valid up to an $E_{max} = 30.58$ eV.

In light of this controversy we have ascribed an uncertainty of 10% in our transmission efficiency determination (Brunger *et al* 1990). This is not a moot point as this uncertainty is a major contributor to the overall uncertainty on the present differential cross section measurements for rovibrationl excitation in H_2. We stress that once this inherent uncertainty in the calibration technique is resolved, or a mechanism is found to specifically calculate the correct yield for a given E_0, then there is no barrier, in principle, to the relative transmission efficiency of the analyser being determined to a high degree of accuracy.

3. Results and discussion

Differential cross sections for elastic scattering and rovibrational excitation of H_2 by electron impact are given in tables 1 and 2 respectively. These differential cross sections have been determined at seven incident electron energies between 1.0 and 5.0 eV, and at scattering angles in the range 5°–130°. The uncertainty in the present measurement of the elastic differential cross section is estimated to be 8% while for the rovibrational differential cross section the uncertainty is estimated to be 14%. A detailed discussion of the components that contribute to these errors and the method of deriving the total uncertainty has been given in Brunger *et al* (1990).

Table 1. Differential cross sections for vibrationally elastic scattering of electrons from H_2 (units are $\times 10^{-16}$ cm^2 sr^{-1}).

	Energy (eV)						
	1.0	1.25	1.5	2.0	2.5	3.0	5.0
Scattering angle (deg)	$\sigma(\theta)$						
20	0.60	0.60	0.78	1.26	1.69	1.97	2.81
30	0.58	0.56	0.72	1.20	1.50	1.70	2.25
40	0.53	0.51	0.66	1.04	1.12	1.37	1.78
50	0.51	0.43	0.61	0.94	0.95	1.21	1.42
60	0.54	0.47	0.62	0.81	0.79	1.07	1.14
70	0.57	0.57	0.70	0.81	0.74	0.84	0.94
80	0.63	0.75	0.79	0.76	0.75	0.75	0.79
90	0.74	0.86	0.92	0.86	0.83	0.79	0.71
100	0.90	1.04	1.12	1.08	0.93	0.99	0.71
110	1.08	1.25	1.28	1.20	1.09	1.18	0.73
120	1.28	1.51	1.46	1.35	1.31	1.28	0.77
130	1.45	1.66	1.63	1.49	1.43	1.41	0.83

In figure 4 we illustrate some representative examples of the present elastic differential cross sections. Also shown in these figures are the most recent calculations of the theoretical groups at the University of Oklahoma and JILA (Snitchler *et al* 1990)—henceforth referred to as the Oklahoma group—and, where applicable, the previous experimental data of Linder and Schmidt (1971), Nishimura *et al* (1985), Shyn and Sharp (1981) and Furst *et al* (1984). The qualitative agreement between the present measurements and the calculation of Snitchler *et al* is good, although there are some

Table 2. Differential cross sections for rovibrational excitation of H_2 by electron impact (units are $\times 10^{-18}$ cm^2 sr^{-1}).

Scatteering angle (deg)	Energy (eV) 1.0	1.25	1.5	2.0	2.5	3.0	5.0
	$\sigma(\theta)$						
5	—	—	4.96	6.86	9.14	9.59	8.19
10	—	2.77	4.74	6.45	8.51	8.73	7.18
20	1.22	2.49	4.30	5.72	7.65	7.79	6.39
30	0.99	2.15	3.65	4.98	6.18	6.28	4.91
40	0.74	1.62	3.23	4.06	4.94	5.29	3.65
50	0.65	1.17	2.79	3.37	4.00	4.47	2.65
60	0.57	0.91	2.39	2.79	3.22	3.52	2.22
70	0.40	0.87	1.91	2.13	2.36	2.88	1.68
80	0.32	0.81	1.61	1.80	1.99	2.13	1.44
90	0.32	0.78	1.45	1.66	1.78	1.76	1.37
100	0.40	0.89	1.36	1.64	1.78	2.17	1.41
110	0.46	1.11	1.44	1.64	1.90	2.65	1.59
120	0.57	1.24	1.59	1.91	2.26	2.85	1.94
130	0.78	1.62	1.78	2.21	2.81	3.48	2.19

quantitative differences. However, we would characterize the overall level of agreement between our experimental results and the theory as being from fair to good across the entire energy range of this study, with the best agreement at higher energies. With respect to previous experimental determinations of the elastic differential cross section, the general level of agreement is good (within the combined uncertainties on the respective sets of data). The exception to this is the work of Nishimura *et al* which clearly does not exhibit the same angular dependence as the other experiments for these cross sections.

Figure 5 illustrates some of the present differential cross sections for rovibrational excitation. Again we can compare the current data with the calculation of Snitchler *et al* where, in this case, we find a good level of agreement for incident electron energies below 2 eV and fair agreement above this energy. A comparison with the previous experimental work of Linder and Schmidt (1971) and Nishimura *et al* (1985) shows that, within the combined uncertainties on the respective sets of data, the agreement between ourselves and Linder and Schmidt is very good while the agreement with Nishimura *et al* is poor. We believe the evidence would strongly suggest that the work of Nishimura *et al* suffered from an angle-dependent effect that was either not recognized or not properly accounted for.

At each energy studied the differential cross sections for elastic scattering and rovibrational excitation were extrapolated to 0° and 180°. This was achieved by using as a guide the appropriate *form* of the respective theoretical cross sections. These data were then integrated to give the total elastic (Q_{el}), total rovibrational (Q_v) and total momentum transfer Q_{MT}^{TOT} cross sections defined by

$$Q_i = 2\pi \int_0^{\pi} \frac{d\sigma}{d\Omega}(\theta)_i \sin\theta \, d\theta \qquad i = \text{el, v} \tag{3}$$

$$Q_{MT} = 2\pi \int_0^{\pi} \frac{d\sigma}{d\Omega}(\theta)_i \sin\theta(1-\cos\theta) \, d\theta \qquad i = \text{el, v} \tag{4}$$

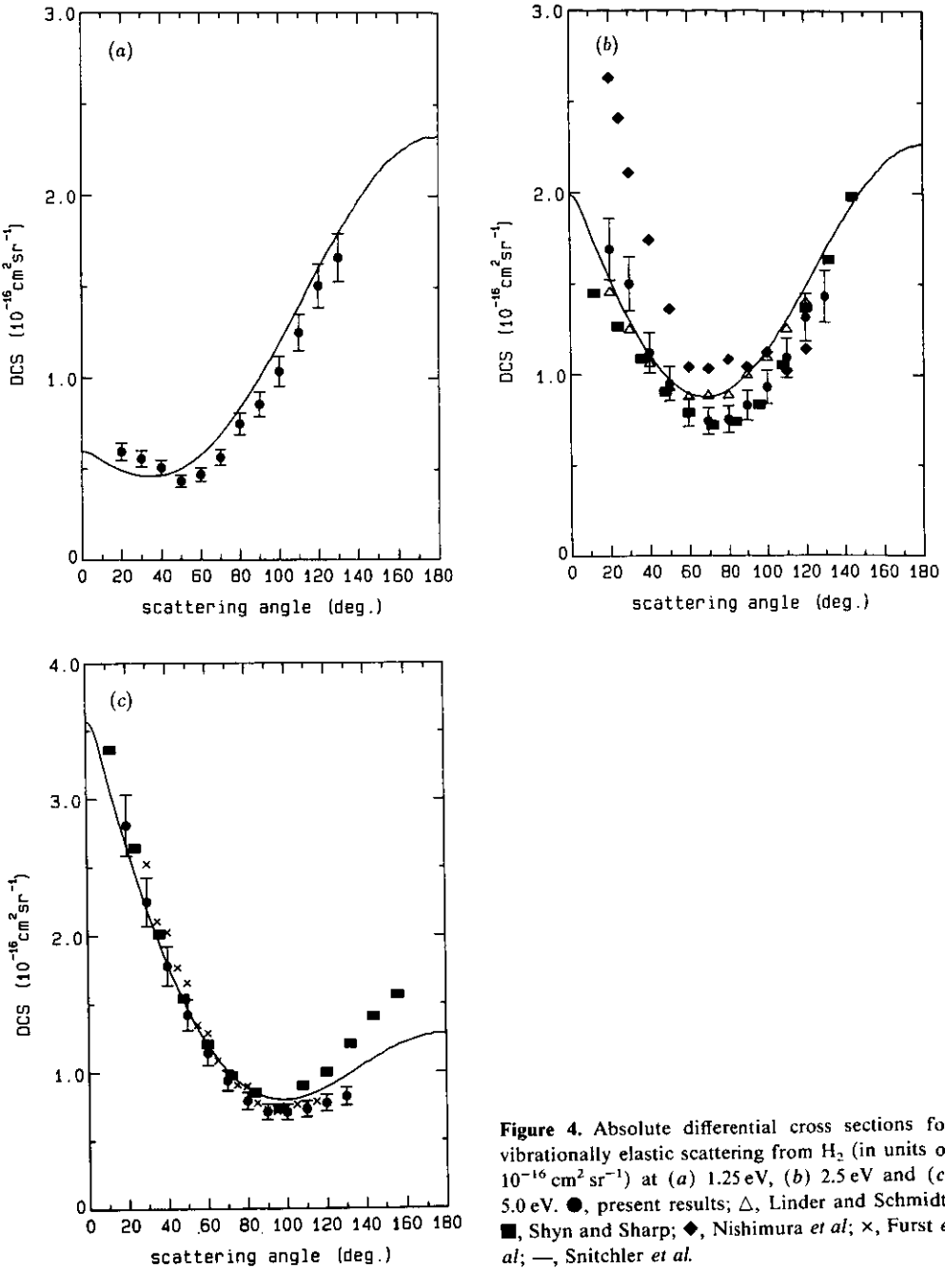

Figure 4. Absolute differential cross sections for vibrationally elastic scattering from H_2 (in units of 10^{-16} cm^2 sr^{-1}) at (*a*) 1.25 eV, (*b*) 2.5 eV and (*c*) 5.0 eV. ●, present results; △, Linder and Schmidt; ■, Shyn and Sharp; ◆, Nishimura *et al*; ×, Furst *et al*; —, Snitchler *et al*.

and

$$Q_{MT}^{TOT} = Q_{MT}^{V} + Q_{MT}^{el}. \tag{5}$$

Values of these cross sections are given in table 3 with the error in each conservatively estimated to be of the order of 20%. This accounts for the uncertainty in the relevant differential cross sections, an uncertainty in the numerical accuracy of the integration

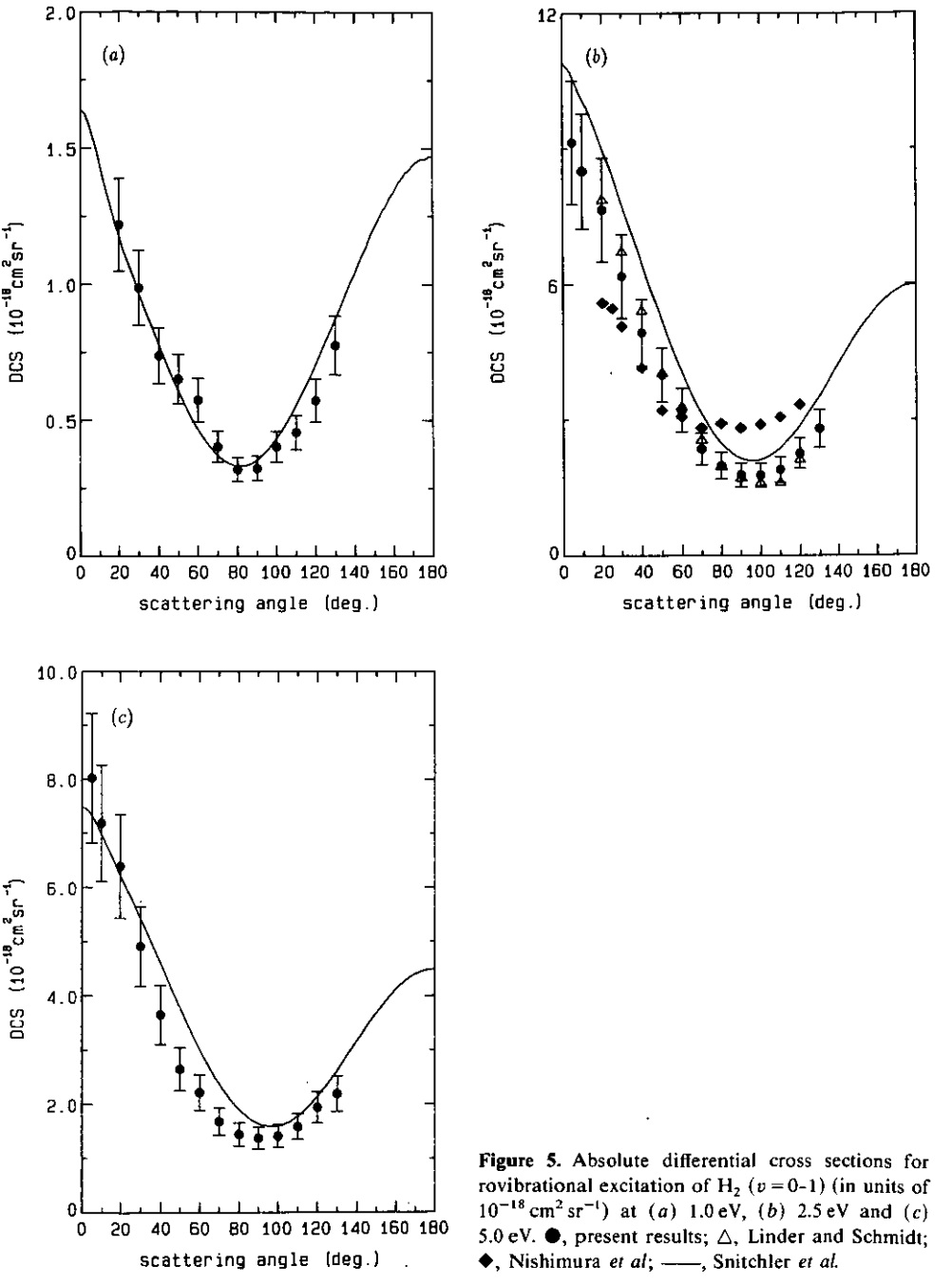

Figure 5. Absolute differential cross sections for rovibrational excitation of H_2 ($v = 0$-1) (in units of 10^{-18} cm^2 sr^{-1}) at (*a*) 1.0 eV, (*b*) 2.5 eV and (*c*) 5.0 eV. ●, present results; △, Linder and Schmidt; ◆, Nishimura *et al*; ——, Snitchler *et al.*

and an uncertainty associated with the extrapolation procedure adopted in the present case.

The present total elastic cross section is shown in figure 6 together with the calculation of Snitchler *et al* (1990) and the experimental results of Furst *et al* (1984), Linder and Schmidt (1971), Nishimura *et al* (1985) and Shyn and Sharp (1981). There is good agreement between the present cross section and the calculation of Snitchler

Table 3. Total elastic, rovibrational and momentum transfer cross sections for the electron impact excitation of H_2 (units are $\times 10^{-16}$ cm^2).

Electron energy	Q_{el}	Q_v	Q_{MT}
1.0	11.68	0.08	14.59
1.25	13.03	0.17	16.84
1.50	13.85	0.25	16.41
2.0	14.56	0.33	16.51
2.5	15.10	0.40	17.11
3.0	15.52	0.46	16.33
5.0	13.90	0.32	11.45

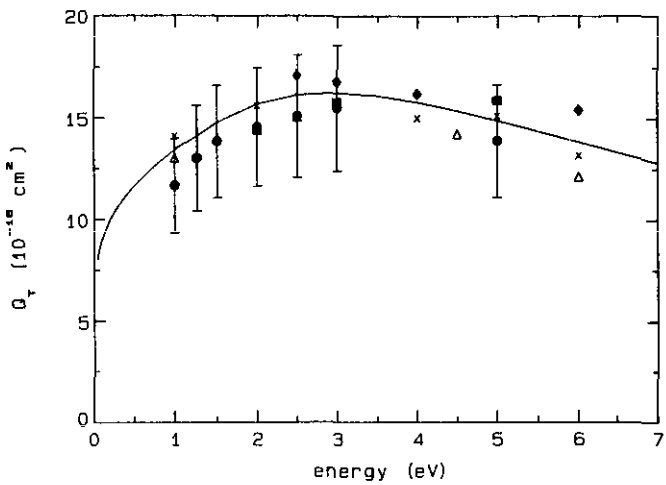

Figure 6. Total cross section for vibrationally elastic scattering from H_2 (in units of 10^{-16} cm^2). ●, present results; △, Linder and Schmidt; ■, Shyn and Sharp; ◆, Nishimura *et al*; ×, Furst *et al*; ——, Snitchler *et al*.

et al, the theoretical curve lying within the experimental error bars at all energies. However, we observe that the present measurement is systematically lower in absolute value, when compared with Snitchler *et al*, across the entire energy regime. There is also substantial overlap, within error limits, between the present measurement and all previous experimental cross sections.

As the backward angle regions (130–180°) which we do not access in the present measurements, make a significant contribution to the total cross section (e.g. about 30% at 2 eV), we have tested the sensitivity of the present total elastic cross sections to our extrapolation procedure by repeating the technique with the form of the elastic differential cross section of Shyn and Sharp as a guide. This was found to yield a value of the total elastic cross section, at 2 eV, which was some 4% higher than that given in table 3. We note here that the total elastic cross section is by far the major contributor to the grand total cross section, at these low energies. The present grand total cross sections (calculated on the basis of $Q_{gt} = Q_{el} + Q_v$ and extrapolating the appropriate differential cross sections with the form of Snitchler *et al*) are given in figure 7 along with the results of the previous time-of-flight experiments of Ferch *et al* (1980) and Jones (1985), the experiment of Subramanian and Kumar (1989) and the calculation

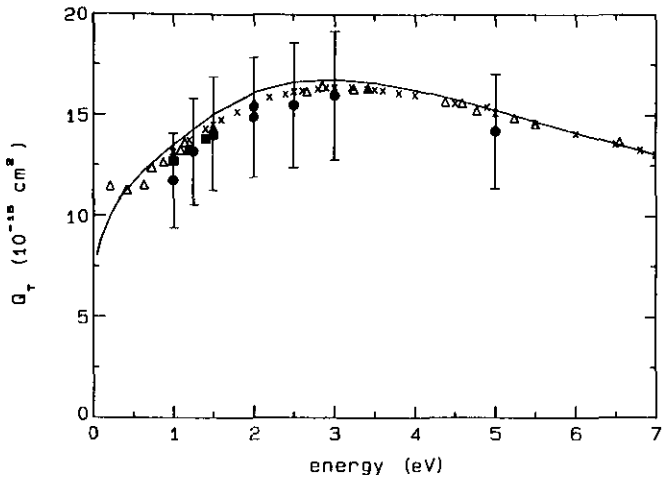

Figure 7. Grand total cross section for electron impact excitation of H_2 (in units of 10^{-16} cm^2). ●, present results; ○, present result using Shyn and Sharp extrapolation (see text); ×, Jones; ■, Ferch *et al*; △, Subramanian and Kumar; ——, Snitchler *et al.*

of Snitchler *et al* (1990). It can be seen that within the uncertainties on our data they are in very good agreement with the earlier measurements and theory. However, for the specific case of 2 eV, we find that the absolute value of the grand total cross section, calculated using an extrapolation based on Shyn and Sharps' elastic differential data, is in significantly better agreement with the values of Jones (1985) and Subramanian and Kumar (1989) (see figure 7; annotation (○)) than that calculated using the form of Snitchler *et al* as a guide in the extrapolation procedure. Also, as the elastic differential cross sections of Shyn and Sharp are always larger at backward angles than those calculated by Snitchler *et al*, the same trend would hold across the energy range of the present study. Whilst one could interpret this observation as evidence that the angular dependence of Snitchler *et al*'s cross section may not be strictly correct at backward angles we prefer to see it as a further justification for the somewhat conservative error limits we have placed on our data as it clearly illustrates the inherent difficulties involved in deriving accurate total cross sections from differential measurements.

Similar comments may be made with respect to the present total momentum transfer cross section. Indeed, given the weighting that this cross section places on collisions in the backward direction, the different extrapolation procedures outlined above are likely to have an even greater effect on the value of the derived momentum transfer cross section. In figure 8 we compare the present Q_{MT}^{TOT} with both the theory and the swarm-derived total momentum transfer cross section of England *et al* (1988). The present data are seen to be in somewhat better agreement with the derived cross section of England *et al* than the calculation of Snitchler *et al* although, within the uncertainty on the present data, there is little to choose between theory and the swarm result. We note that the tabulated momentum transfer cross section of England *et al* shows a discontinuity at energies above 5 eV. Elford (1990) has indicated that, as a consequence of uniqueness problems in the swarm analysis, this cross section is only reliable at energies below 5 eV.

Figure 9 presents the measured rovibrational ($v = 0 \rightarrow 1$) integral excitation cross section. Here we observe fair overall agreement with the calculation of Snitchler *et al*

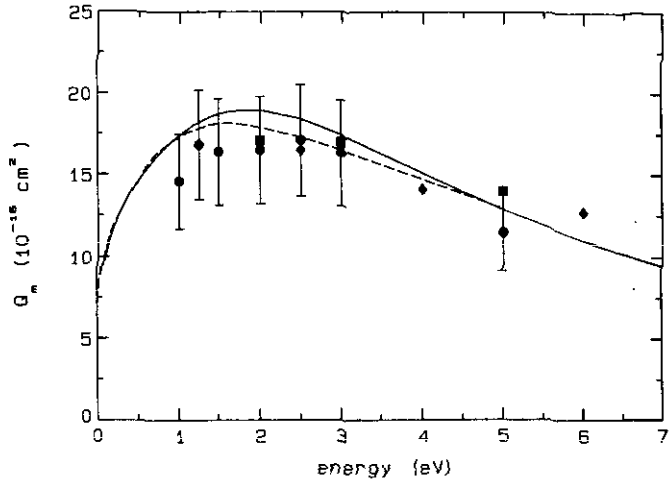

Figure 8. Total momentum transfer cross section of H_2 (in units of 10^{-6} cm^2). ●, present results; ■, Shyn and Sharp; ◆, Nishimura *et al*; ——, Snitchler *et al*; - - - -, England *et al.*

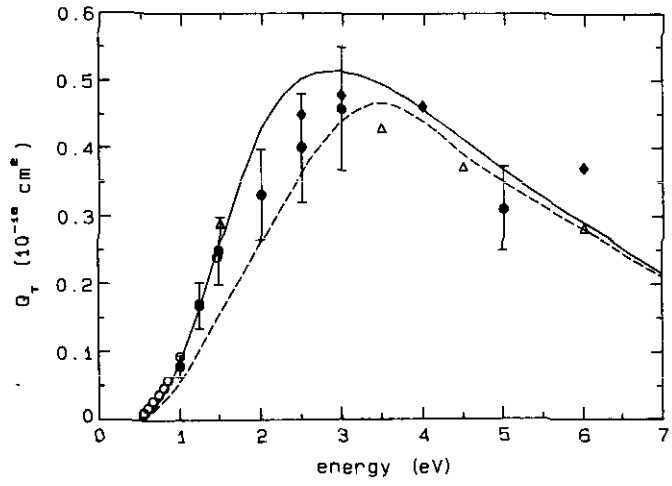

Figure 9. Total cross section for rovibrational excitation ($v \approx 0$–1) of H_2 (units of 10^{-16} cm^2). ●, present results; △, Linder and Schmidt; ◆, Nishimura *et al*; ○, Ehrhardt *et al*; ——, Snitchler *et al*; - - - -, England *et al.*

although we highlight the very good agreement between the present data and theory for energies below 2 eV. In this same energy regime the present integral cross section is clearly not compatible with the swarm-derived cross section of England *et al* (1988). This point has been discussed in detail elsewhere (Buckman *et al* 1990) but we again emphasize our belief that this is an important result which has ramifications for either the swarm analysis of transport parameters or for both the theoretical formalism of the Oklahoma group and the present experiments.

The current data is also found (see figure 9) to be in good agreement in terms of the absolute value of the cross section, and the position of the peak in the cross section,

with the previous beam measurements of Ehrhardt *et al* (1968), Linder and Schmidt (1971), Allan (1985) and Nishimura *et al* (1985) although the agreement with Nishimura is probably fortuitous as the shape of their differential cross section is clearly at variance with our results, the theory, and with Linder and Schmidt (see figure 5(*b*)).

4. Conclusions

The present elastic and rovibrational differential cross sections and the corresponding total elastic, rovibrational and momentum transfer cross sections provide a significant volume of data against which the Oklahoma group can test their most recent calculations for low energy electron–H_2 scattering. In making these comparisons we found that, whilst there were differences in some details, the level of agreement was, in general, good and thus should provide them with some assurance when applying their model to low energy electron scattering from other collision systems of interest.

The present data also provide, along with previous beam determinations, further evidence that the near-threshold impasse between theory and the swarm derived integral cross section for rovibrational excitation should be resolved in favour of the theory.

We are not qualified to make any detailed observations on either the swarm experiments or, in particular, the analysis of the transport coefficients which is required to obtain a set of scattering cross sections. However, given the extent of the disagreement on this most fundamental problem and the ramifications it may have for the techniques used to obtain the vibrational excitation cross section, some detailed general comments are warranted. Firstly, the conceptually simple nature of the swarm experiments, and the good agreement that exists between swarm-derived momentum transfer cross sections, theory and beam experiments for a simple atomic target such as helium, suggest that the swarm *experiments* themselves are unlikely to be in error. Nonetheless, to our knowledge there are no independent experimental data available for H_2 and this would clearly be desirable to remove any possible doubts concerning the accuracy of the measured transport coefficients. Such a suggestion has already been made by Morrison *et al* (1987). Secondly, and more importantly, we would emphasize the need for an alternative method of analysis of the experimental transport data to be undertaken. Such a programme, using Monte Carlo techniques to provide an independent check of the present conventional transport theory, is already planned (Brennan 1990). We also feel that it would be most instructive if an accurate estimation of the degree of uniqueness of the swarm-derived cross section set could be provided through a rigorous error analysis conducted in conjunction with the transport analysis. Error bounds on the derived cross sections would enable an accurate assessment of the level of disagreement to be made.

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References

Allan M 1985 *J. Phys. B: At. Mol. Phys.* **18** L451
Brennan M J 1990 Private communication
Brunger M J, Buckman S J and Newman D S 1990 *Aust. J. Phys.* **43** 665
Buckman S J, Brunger M J, Newman D S, Snitchler G, Alston S, Norcross D W, Saha B, Danby G, Trail W and Morrison M A 1990 *Phys. Rev. Lett.* **65** 3253
Crompton R W, Gibson D K and Robertson A G 1970 *Phys. Rev.* A **2** 1386
Ehrhardt H, Langhans L, Linder F and Taylor H S 1968 *Phys. Rev.* **173** 222
Elford M T 1990 Private communication
England J P, Elford M T and Crompton R W 1988 *Aust. J. Phys.* **41** 573
Ferch J, Raith W and Schroder K 1980 *J. Phys. B: At. Mol. Phys.* **13** 1481
Furst J, Mahgerefteh M and Golden D E 1984 *Phys. Rev.* A **30** 2256
Hammond P, Read F H, Cvejanovic S and King G C 1985 *J. Phys. B: At. Mol. Phys.* **18** L141
Henry R J W and Lane N F 1969 *Phys. Rev.* **183** 221
Jones R K 1985 *Phys. Rev.* A **31** 2898
Keenan G A, Walker I C and Dance D F 1982 *J. Phys. B: At. Mol. Phys.* **15** 2509
Khakoo M A and Trajmar S 1986 *Phys. Rev.* A **34** 138
Linder F and Schmidt H 1971 *Z. Naturforsch.* **26a** 1603
Morrison M A, Feldt A N and Saha B C 1984 *Phys. Rev.* A **30** 2811
Morrison M A, Crompton R W, Saha B C, Petrovic Z Lj 1987 *Aust. J. Phys.* **40** 239
Nesbet R K 1978 *Phys. Rev.* A **20** 58
Nickel J C, Zetner P W, Shen G and Trajmar S 1989 *J. Phys. E: Sci. Instrum.* **22** 730
Nishimura H, Danjo A and Sugahara H 1985 *J. Phys. Soc. Japan* **54** 1757
Pichou F, Huetz A, Joyez G and Landau M 1978 *J. Phys. B: At. Mol. Phys.* **11** 3683
Schubert E, Jung K and Ehrhardt H 1981 *J. Phys. B: At. Mol. Phys.* **14** 3267
Shyn T W and Sharp W E 1981 *Phys. Rev.* A **24** 1734
Snitchler G, Alston S, Norcross D, Saha B, Danby G, Trail W and Morrison M A 1990 Private communication
Sohn W K, Jung K and Ehrhardt H 1983 *J. Phys. B: At. Mol. Phys.* **16** 891
Srivastava S K, Chutjian A and Trajmar S 1975 *J. Chem. Phys.* **63** 2659
Subramanian K P and Kumar V 1989 *J. Phys. B: At. Mol. Opt. Phys.* **22** 2387