J. Phys. B: At. Mol. Opt. Phys. 26 (1993) 121–128. Printed in the UK

Differential cross sections for elastic scattering of electrons from N_2 at 0.55, 1.5 and 2.2 eV

Xueying Shi, T M Stephen† and P D Burrow

Department of Physics and Astronomy, University of Nebraska, Lincoln, NE 68588, USA

Received 5 June 1992

Abstract. Differential cross sections for vibrationally elastic scattering of electrons from N_2 have been measured at three energies using the relative flow technique and normalizing to the cross sections in helium. At 1.5 eV our results generally support the recent observations of Brennan *et al*, who find substantially larger cross sections than previously reported by Shyn and Carignan and by Sohn *et al*. At 0.55 eV, our results are also larger than those of Sohn *et al*, but in good agreement with the calculations of Morrison *et al*. A measurement is also reported at the second peak of the $^2\Pi_g$ temporary negative ion state, and several difficulties in making comparisons with theory and experiment are elucidated.

Brennan *et al* (1992) have recently reported a differential cross section for the scattering of electrons from N_2 at 1.5 eV which differs substantially in magnitude from the two previous measurements by Shyn and Carignan (1980) and Sohn *et al* (1986). During the course of testing our apparatus at low energies, we also encountered such a discrepancy. We have further extended our study to lower energy, 0.55 eV, and again find a difference with the work of Sohn *et al* which is outside the quoted range of experimental error. In this paper we also report a measurement in the region of the $^2\Pi_g$ resonance and comment on some problems which make close comparisons of experimental and theoretical results difficult.

Our electron scattering apparatus has been briefly described in Stephen and Burrow (1991), a study of vibrational excitation in 1,4-cyclohexadiene. The provisions for making absolute cross section measurements using the relative flow method (see Nickel *et al* 1989 and references therein) are outlined in Shi and Burrow (1992). This latter study describes measurements of the differential cross section in neon from 7 eV down to 0.25 eV. Because of the excellent agreement between our electron beam measurements, recent *ab initio* theoretical results and with cross sections derived from swarm measurements, we have suggested that neon is a useful secondary standard with which to verify the performance of the apparatus. We have used these studies to gain assurance that systematic errors in the present work are small.

In the present work on N_2, we have employed the relative flow technique using helium as a calibrant and normalized to the cross sections of Nesbet (1979). We have adjusted the ratio of the flow rates to within 20% of the value which sets the Knudsen numbers of both gases equal at the entrance to the gas needle. As described elsewhere (Nickel *et al* 1989) this causes the angular distribution of the gases leaving the needle to be the same. In our apparatus, an internal four-port switch directs the target gas to the needle and helium into the background, or the reverse. Thus, both gases are present

† Present address: Department of Physics, University of Denver, Denver, CO 80208, USA.

at all times in the background and contact potential shifts are minimized in switching between gases. Careful account of the scattering off the background gases is made by directing both gases into the background and subtracting this contribution from the signal. The energy scale is calibrated by reference to the resonance structure of N_2 in the 2 eV region using the values given by Rohr (1977). The overall energy resolution in this experiment is approximately 30 meV, full width at half maximum.

In the data to be shown, normalization to the helium cross section was carried out at each angle shown, for a given impact energy. To give a better idea of the overall reproducibility of the experiment, each point represents the average of measurements taken on several different days. The error brackets indicate ± the standard deviation of these values. To avoid cluttering the figures, only a single bracket is shown with the understanding that the same percentage deviation exists at the other points, unless otherwise noted.

As noted by Brennan *et al*, there are few absolute measurements of the differential elastic scattering cross section in N_2 below the 2 eV resonance region. At the lowest energy we have examined, 0.55 eV, we are only aware of the work of Sohn *et al* (1986). Figure 1 shows the angular distribution measured in the present work and that of Sohn *et al*. The full curve shows the differential elastic cross section from the calculations of Morrison *et al* (1987) using a parameter-free model polarization potential. As the scattering angle increases, the present data systematically depart from those of Sohn *et al*, which lie some 27% lower at 120°. On the other hand, agreement with the calculations of Morrison *et al* is exceptionally good below 80°. Between 80° and 120°, the present data are about 8–12% higher, with the theoretical data lying just outside the standard deviation. Since rotational excitation is not resolved in the present study, it would be more appropriate to compare our results with the cross section for

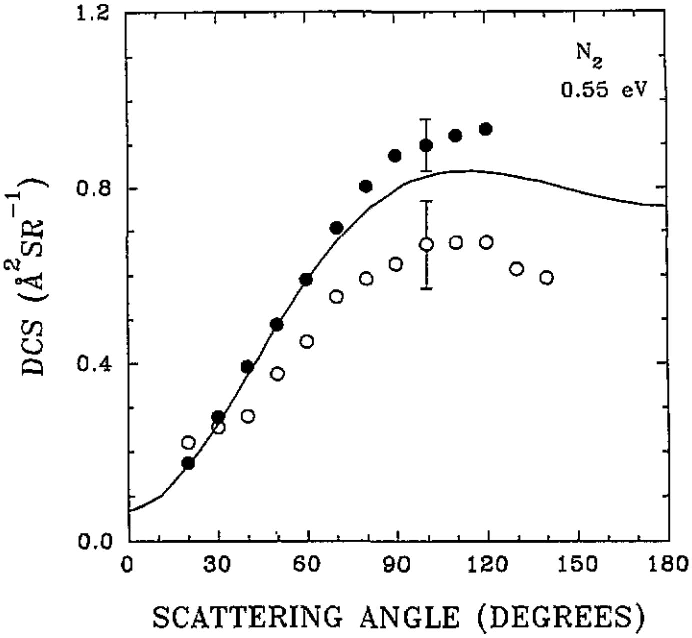

Figure 1. The differential vibrationally elastic scattering cross section of N_2 at 0.55 eV. Present data, full circles; Sohn *et al*, open circles; Morrison *et al*, full curve.

differential elastic scattering plus rotational excitation. According to Morrison *et al*, the angle-integrated total cross section including rotation is 3.4% higher than the integrated purely elastic cross section. This further improves the agreement between theory and our experiment.

By extrapolating our data to 0° and 180°, using the curve of Morrison *et al* as a guide, we find an integrated vibrationally elastic cross section of 9.24 Å^2 at 0.55 eV. Table 1 shows a comparison with the experimental total cross sections of Kennerly (1980) and Baldwin (1974) as well as the result of Morrison *et al* and the angle-integrated cross section of Sohn *et al*. The present result is only 2% above that of Baldwin and 3.9% above Kennerly. Uncertainties in these latter experiments are ±1–2% and ±3% respectively, and considering the standard deviation of ±6% in the present experiment, the overall agreement is quite satisfactory.

Figures 2 and 3 compare the present data at 1.5 eV with existing experimental data and a selection of theoretical values, respectively. The experimental data points are

Table 1. Total and integrated vibrationally elastic cross sections of electrons from N_2.

	σ_{total} (Å^2)		$\sigma_{\text{int.vib.el.}}$ (Å^2)			
Energy (eV)	Baldwin	Kennerly	Present work	Sohn *et al*	Brennan *et al*	Morrison *et al*
0.55	9.05	8.896	9.24	6.81	—	8.81
1.50	11.6	11.17	11.6	7.43	12.7	11.50

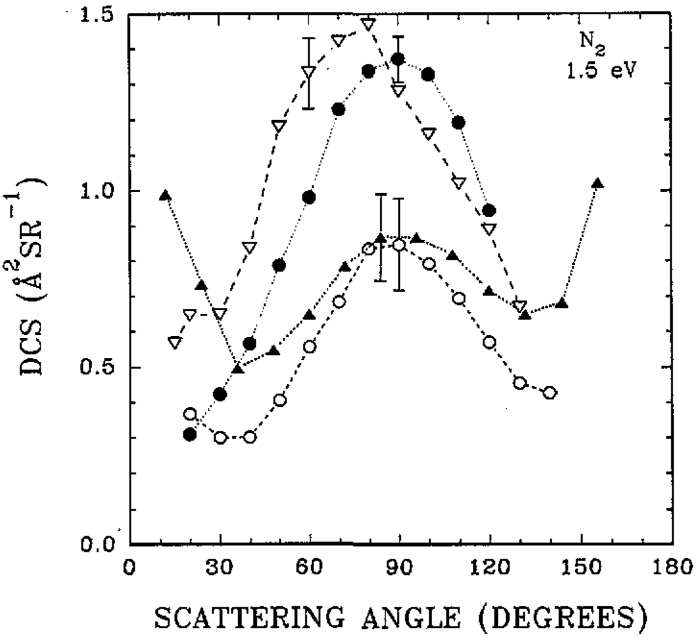

Figure 2. The differential vibrationally elastic scattering cross section of N_2 at 1.50 eV determined by experiment. Present data, full circles; Brennan *et al*, open triangles; Sohn *et al*, open circles; and Shyn and Carignan, full triangles. The data points are connected with straight line segments to guide the eye.

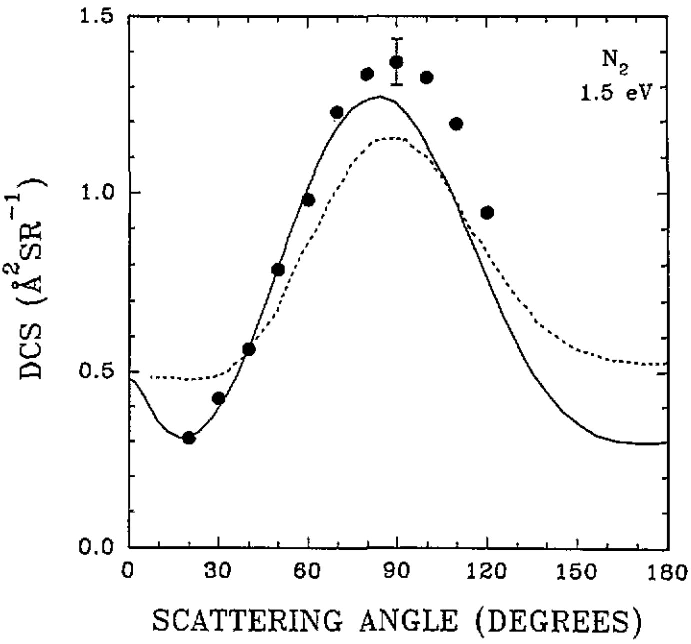

Figure 3. The differential vibrationally elastic scattering cross section of N_2 at 1.50 eV. A comparison of the present results, full circles, with theoretical calculations by Huo *et al* (broken curve) and Morrison *et al* (full curve).

connected with straight line segments to guide the eye. Representative uncertainties are shown for each set of data. The present work confirms the observation of Brennan *et al* with regard to the cross section near 90° which is approximately 50% larger than those observed by Shyn and Carignan and Sohn *et al.* The latter two studies are in surprisingly close agreement near 90°, a concurrence that perhaps inhibited other measurements at this energy. The cross sections differ substantially at larger and smaller angles, however. The present data show no evidence for the pronounced rise in cross section observed by Shyn and Carignan at small angles, or even the more modest rise in the data of Sohn *et al.* The curve of Brennan *et al* does not show an increase and thus is consistent with the present data. We cannot measure beyond 120° so the increase at large angles cannot be checked.

Unfortunately there are still significant differences between the data of Brennan *et al* and the present work which are well outside the range of uncertainties. The two curves appear to be shifted from one another by 10°–15°, a much larger amount than can be accounted for by errors in angular positioning. Brennan *et al* determine their zero angle by observing the symmetry in elastic scattering around the forward direction and quote an estimated error of ±1°. We rely on the mechanical alignment of our apparatus to determine the 0° setting, which is consistent also with the primary electron beam direction. The alignment is unchanged from our measurements in neon. If there is in fact an angular error in that study, it would suggest that our data should be shifted to higher angles rather than lower. The sources of the differences between the four sets of data at 1.5 eV are unclear but the comparison amply indicates that systematic errors have been largely underestimated at low electron energies.

Brennan *et al* have carried out a more exhaustive comparison of their data with theory. In this paper, we restrict ourselves in figure 3 to the Schwinger multichannel calculations of Huo *et al* (1987) and the results of Morrison *et al.* Again the cross section of the latter is in good agreement with the present data, particularly at angles below 80°. The inclusion of rotational excitation would improve the agreement further.

Integration of our angular data, again following the theoretical curve of Morrison *et al* as a guide, yields a total cross section of 11.6 Å^2, assuming that vibrational excitation is a negligible contributor at 1.5 eV. As shown in table 1, this value lies 3.9% above that of Kennerly but is coincident with that of Baldwin. The integrated total cross section for elastic scattering and rotational excitation of Morrison *et al* lies less than 1% below the present data. The integrated vibrationally elastic cross section measured by Brennan *et al* is 12.7 Å^2 which lies 9.5% above the present cross section.

Cross section measurements in the region of the $^2\Pi_g$ resonance of N_2 present a number of problems, particularly with regard to making close comparisons with other experimental data and with theory. The primary problem has been well recognized, namely that the rapid variations in the scattering cross section due to the presence of the 'quasivibrational' levels of the temporary negative ion state make small differences in the energy of measurement important. Less well appreciated are effects arising from the angular dependence of the peak energies in the elastic scattering; see Rohr (1977) for example. Thus, the early measurements of Shyn and Carignan reported differential cross sections at the lowest three peaks in the resonance scattering, which were located at 1.9, 2.1, and 2.4 eV as observed at a scattering angle of 144°. At this angle, the differential cross sections have close to their minimum values. At small angles where the cross sections are much larger, the peaks occur at 1.947, 2.215 and 2.467 eV, according to Rohr's data at 20°. Setting the impact energy to the peak at a large angle will thus cause the low angle scattering to be underestimated with respect to measurements in which the peak is located at small angles.

Comparison with theory now adds an additional twist to the story. Huo *et al* calculated their cross sections at the energies given by Shyn and Carignan, 2.1 eV in the case of the second peak to which we restrict our discussion. However this energy did not coincide with the energy of their calculated peak. Rather, it lies 87 meV below the peak in the total cross section which they find at 2.187 eV†.

Finally, to complete the circle, the recent measurements of Brennan *et al* were carried out at 2.1 eV because of the existing theoretical and experimental values at this energy, and without any particular regard to the energy of the resonance peak. In any case, differences in energy calibration among the various experimental groups may also cause additional discrepancies to further confuse the issue.

The effects described above suggest a protocol for displaying the differential data for purposes of comparison which eliminates all problems with energy calibration and the variation of peak energy with angle. We propose simply to adjust the impact energy at each angle by the small amount necessary to stay on the local maximum in the cross section. Such an 'impact energy optimized' differential cross section could also be generated theoretically to obviate shifts in the computed resonance energies.

We have carried out such a measurement for the second resonance peak, corresponding to $v'=1$ of the quasivibrational levels of the $N_2^-(^2\Pi_g)$ state, which occurs at 2.219 eV in the total cross section measurement of Kennerly (1980). Because of the significant rotational excitation taking place through the resonance, normalization to the He cross section was carried out by careful integration of the entire elastic beam profiles in both N_2 and He.

† Private communication, Dr Winifred Huo.

Our 'energy optimized' differential cross section at the nominally 2.22 eV peak is shown in figure 4. Strictly speaking, these results cannot be matched directly with any published data. However a reasonably close comparison can be made with the data of Jung *et al* (1982) shown as a full curve. These data were acquired at a fixed impact energy of 2.22 eV, which is coincident with the peak energy at 20° reported by Rohr, also at the same institution. The overall agreement is quite good although there are differences near the minimum at 60° which is less pronounced in the data of Jung *et al.* The differential cross section in the present work increases more rapidly as the scattering angle is decreased. This is likely due to our 'tracking' along with the peak at these low angles where the cross section is large.

The data of Brennan *et al* and the theoretical curve of Huo *et al* were determined at a fixed impact energy of 2.1 eV and are therefore not directly comparable to the other data. Not surprisingly they fall below at all angles. As a rough check to verify the difference between these data and those of the present work, we measured at 30° the ratio of the differential cross section at the peak energy minus 87 meV, as in the calculation of Huo, to the cross section at the peak. This information suggests that the cross section of Huo *et al* would be approximately 1.5 times larger at this angle if it had been calculated at the peak, which places the cross section in much better agreement. A roughly similar 'optimization' pertains also to the 2.1 eV data of Brennan *et al.*

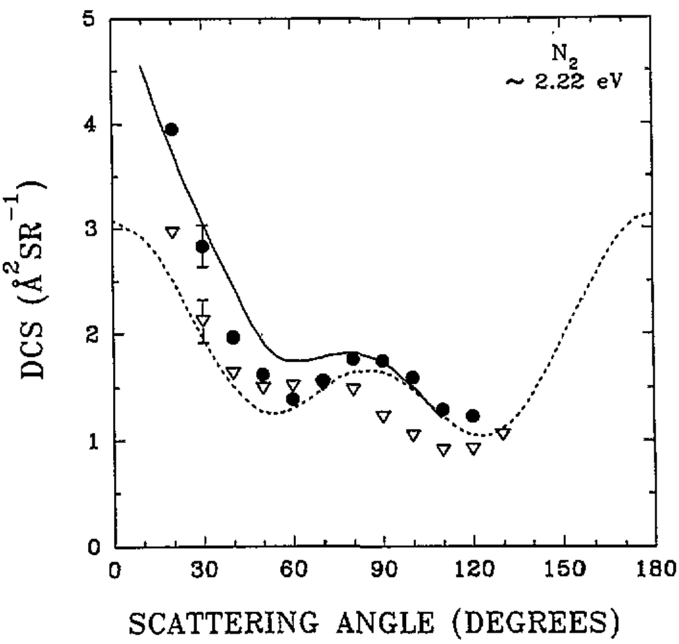

Figure 4. The differential vibrationally elastic scattering cross section of N_2 at or near 2.22 eV, the second peak of the $N_2^-(^2\Pi_g)$ resonance. The present data (full circles), are acquired by readjusting the impact energy slightly at each angle to stay on the peak. The results of Jung *et al* (full curve) are taken at a fixed energy of 2.22 eV, the data of Brennan *et al* (open triangles), at a fixed energy of 2.1 eV, and the theoretical curve by Huo *et al* (broken curve) at a fixed energy of 2.1 eV, 87 meV below the resonance peak in their calculations.

Table 2. The differential vibrationally elastic scattering cross sections ($Å^2\,sr^{-1}$), of electrons from N_2 as a function of angle.

Angle	0.55 eV	1.50 eV	2.2 eV†
20	0.175	0.310	3.95
30	0.280	0.424	2.83
40	0.393	0.566	1.97
50	0.490	0.788	1.62
60	0.590	0.981	1.39
70	0.706	1.228	1.56
80	0.803	1.337	1.76
90	0.875	1.371	1.75
100	0.898	1.327	1.59
110	0.921	1.193	1.29
120	0.935	0.945	1.23
Standard deviation	±6%	±6%	±8%

† The impact energy has been adjusted to the peak energy at each angle as described in the text.

Table 2 lists all our differential cross section data. The bottom line in this table gives the standard deviation of each of the data sets.

In conclusion, systematic errors in the measurement of differential cross sections in N_2 at energies below approximately 2 eV appear to be larger than recognized by most practitioners. This is surprising since most studies normalize to the helium cross section using the relative flow method, and one would expect that many experimental parameters, which by themselves would be difficult to determine, would cancel out in the final cross section ratio. Our approach to this has been to verify that our apparatus and the methods of operation reproduce the known neon cross section to an acceptable degree, in our case better than 3%. We must note however that while this will give confidence regarding many aspects of the cross section measurement, there are other points, such as setting the proper flow rates in gases which are much heavier than helium, which still may produce systematic errors.

Finally, we have made some suggestions regarding the measurement of the cross section at energies where the scattering varies rapidly, which should permit more accurate comparisons of theory and experiment to be made.

Acknowledgments

This work was supported by NSF through grant CHE-8922601. The authors thank Dr S J Buckman for several useful conversations and a preprint of the work of Brennan *et al.*

References

Baldwin G C 1974 *Phys. Rev.* A **9** 1225

Brennan M J, Alle D T, Euripides P, Buckman S J and Brunger M J 1992 *J. Phys. B: At. Mol. Opt. Phys.* **25** 2669

Huo W M, Lima M A P, Gibson T L and McKoy V 1987 *Phys. Rev.* A **36** 1642

Jung K, Antoni Th, Müller R, Kochem K-H and Ehrhardt H 1982 *J. Phys. B: At. Mol. Phys.* **15** 3535
Kennerly R E 1980 *Phys. Rev.* A **21** 1876
Morrison M A, Saha B C and Gibson T L 1987 *Phys. Rev.* A **36** 3682
Nesbet R K 1979 *Phys. Rev.* A **20** 58
Nickel J C, Zetner P W, Shen G and Trajmar S 1989 *J. Phys. E: Sci. Instrum.* **22** 730
Rohr K 1977 *J. Phys. B: At. Mol. Phys.* **10** 2215
Shi X and Burrow P D 1992 *J. Phys. B: At. Mol. Opt. Phys.* **25** 4273
Shyn T W and Carignan G R 1980 *Phys. Rev.* A **22** 923
Sohn W, Kochem K-H, Scheuerlein K-M, Jung K and Ehrhardt H 1986 *J. Phys. B: At. Mol. Phys.* **19** 4017
Stephen T M and Burrow P D 1991 *Chem. Phys. Lett.* **179** 252