Experimental differential and integral electron impact cross sections for the B $^1\Sigma_u^+$ state of H_2 in the intermediate-energy region†

Santosh K Srivastava and Stephen Jensen‡

Jet Propulsion Laboratory, California Institute of Technology, Pasadena, California 91103, USA

Abstract. Utilising a crossed electron-beam–molecular-beam scattering technique, differential electron impact cross sections (DCS) for the excitation of the $v' = 2$ vibrational band of the B $^1\Sigma_u^+$ state of H_2 have been measured and are presented for the first time. These measurements were made at electron impact energies of 15, 20, 30, 40, 50 and 60 eV. At each energy, DCS between scattering angles of 10° and 135° were determined. They were then extrapolated to 0° and 180° scattering angles to obtain the integral cross sections. These integral cross sections and the Frank–Condon factor for the $v' = 2$ band were used to calculate the total cross sections for the excitation of the B $^1\Sigma_u^+$ state.

1. Introduction

Electron impact excitation cross sections of the B $^1\Sigma_u^+$ state of H_2 are not available. From the practical point of view, this state is important because it gives rise to the Lyman band system in the vacuum ultraviolet (VUV) region of the spectrum and is largely responsible for the Lyman-α radiation which results when H_2 is excited by electron impact. In addition to this, H_2, being the simplest molecule, is of special interest for testing theoretical calculations.

In this paper, we present the following cross sections for intermediate electron impact energies: (a) differential cross sections (DCS) $\sigma_{v' = 2}$ for scattering angles between 10° and 135°; (b) integral cross sections σ_I for excitation of the $v' = 2$ band of the B $^1\Sigma_u^+$ state; and (c) total cross sections σ_T for excitation of the B $^1\Sigma_u^+$ state of H_2 from its ground state. In §2, details of the apparatus and method used are given and in §3 results are discussed.

2. Apparatus and method

2.1. Apparatus

The electron impact spectrometer and its electron optics used in the present measurements have been described in detail elsewhere (Chutjian 1974, Srivastava et al 1975a).

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‡ Permanent address: Physics Department, University of California, Riverside, California 92502, USA.

A crossed electron-beam–molecular-beam scattering geometry (Srivastava *et al* 1975a) was utilised. An energy-selected electron beam (0·035 to 0·050 eV FWHM) was produced by passing the electrons emitted from a heated tungsten filament through a hemi-spherical analyser. The electron beam was focused on the molecular-hydrogen beam which was produced by passing a research-grade H_2 gas through a stainless-steel capillary array. Electrons scattered at an angle θ were accepted by an electron energy analyser. This analyser had electron optics which were similar to those used in producing the electron beam. A spiraltron, a fast pulse amplifier, and a multichannel scalar were used for detecting and counting the scattered electrons. The entire spectrometer was sufficiently stable in its operation so that data could be acquired continuously over a period of 48 hours without any noticeable drift in the scattered-electron signal.

The following steps were taken to ensure the accuracy of the experiment and to minimise possible errors.

(i) The incident-electron-beam energy was calibrated by observing the 19·36 eV resonance in helium.

(ii) The angle $\theta = 0$ was determined by observing the symmetry of the 2^1P excitation of helium.

(iii) At small angles there was a possibility that the direct beam would be detected and hence would make a spurious contribution to the elastic-scattering intensity. To check this, the H_2 beam was turned off and the direct beam was monitored as a function of angle. For angles of 10° or larger, it was found that the direct-beam contribution was insignificant ($< 0.1\%$).

(iv) Possible changes in the transmission efficiency of the detector as a function of energy loss were minimised by varying the potentials on the various electron lenses in the detector as the energy-loss spectrum was swept. In this manner, the
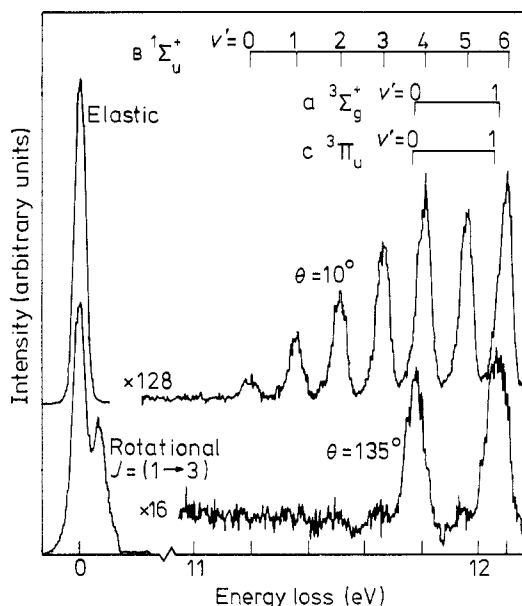

Figure 1. Energy-loss spectra of H_2 for an electron impact energy of 20 eV and scattering angles of 10° and 135°.

transmission efficiency was held at an optimum value at both the elastic peak and at the B $^1\Sigma_u^+$ ($v' = 2$) excitation.

(v) The experiments were repeated after a period of a few months, during which time the electron optics were cleaned and realigned, and the spectrometer was calibrated. It was found that, within the limits of the experimental errors, the results were reproducible.

2.2. *Method*

Energy-loss spectra were obtained at each scattering angle and impact energy. Figure 1 shows two such energy-loss spectra, one at 10° and the other at 135° scattering angle. Each spectrum consists of a spectral feature which corresponds to the elastically scattered electrons and several other features which are vibrational bands of the B $^1\Sigma_u^+$ state. These spectra were obtained by first scanning through the elastic feature and then jumping to an energy loss of 10·9 eV and scanning to an energy loss of 12·1 eV. At large angles, triplet states (figure 1) tended to dominate the inelastic spectra and this occurrence necessitated the choice of the $v' = 2$ vibrational excitation as the one on which to perform the DCS measurements. Also, at large angles, the elastic feature is seen to consist of rotational excitation as well as the elastic peak (Srivastava *et al* 1975b). Similar spectra were obtained at other scattering angles and electron impact energies.

At each electron impact energy and at each scattering angle, the areas under both the elastic feature and the inelastic peak corresponding to the vibrational band $v' = 2$ were measured by a planimeter. These areas are directly proportional to their respective scattering intensities and thus the ratios $I_{v'=2}/I_{00}$ may be obtained. Here $I_{v'=2}$ is the scattering intensity for the vibrational band $v' = 2$ and I_{00} is the intensity for the elastic scattering. The electron optics in the analyser were compensated in such a way that the electron transmission efficiency remained the same for both elastically scattered electrons as well as for inelastically scattered ones. Thus, these ratios are directly proportional to the ratios of their cross sections, $\sigma_{v'=2}/\sigma_{00}$, where $\sigma_{v'=2}$ is the DCS for the $v' = 2$ band and σ_{00} is the DCS for the elastic scattering. The values of σ_{00} have been published previously (Srivastava *et al* 1975a). These ratios were multiplied by the known σ_{00} values, thus producing absolute values of $\sigma_{v'=2}$.

3. Results and discussion

Differential cross sections $\sigma_{v'=2}$ are presented in table 1 for electron impact energies of 15, 20, 30, 40, 50 and 60 eV and for scattering angles ranging from 10° to 135°. In figures 2(*a*) and 2(*b*), their angular distributions are plotted. Since there are no theoretical results or any other guide presently available, below 10° and above 135° scattering angles these angular distribution curves were extrapolated to 0° and 180° respectively. In the past, for the purpose of extrapolations, two extreme methods have been employed (Trajmar *et al* 1970). In the first method, straight lines parallel to the *x*-axis are drawn from the data points at 10° and 135° respectively. The integral cross sections obtained in this way are certainly too low. The second method uses the extrapolation which has a slope five times as steep as the one measured between the last two data points. In the case of present measurements, the second method

Table 1. Differential cross sections ($\sigma_{v'=2}$), integral cross sections ($\sigma_I(v'=2)$) and total cross sections (σ_T) for the electron impact excitation of the B $^1\Sigma_u^+$ state at different scattering angles θ and incident electron energies E_0.

| E_0 (eV)	$\sigma_{v'=2}$ (10^{-24} m² sr⁻¹)									$\sigma_I(v'=2)$ (10^{-24} m²)	σ_T (10^{-21} m²)
θ (deg) =	10	20	30	40	50	70	90	115	135		
15	14 ± 4·2	8·0 ± 1·8	5·6 ± 1·7	5·0 ± 1·3	4·4 ± 1·1	3·3 ± 0·9	3·2 ± 1·0	3·6 ± 1·3	4·2 ± 1·5	52 ± 15	1·4 ± 0·4
20	38 ± 9·1	21 ± 5·0	11 ± 2·9	6·2 ± 1·6	4·9 ± 1·5	3·6 ± 1·3	3·8 ± 1·1	4·0 ± 1·5	7·2 ± 4·0	71 ± 21	1·9 ± 0·6
30	100 ± 22	33 ± 7·9	15 ± 3·6	7·1 ± 1·8	4·7 ± 1·2	3·5 ± 0·9	2·4 ± 0·7	1·5 ± 0·5	1·1 ± 0·5	74 ± 22	2·0 ± 0·6
40	170 ± 40	41 ± 9·8	12 ± 3·1	4·0 ± 1·2	3·0 ± 0·9	1·9 ± 0·6	1·5 ± 0·6	0·96 ± 0·44	0·81 ± 0·44	85 ± 25	2·3 ± 0·7
50	250 ± 60	52 ± 12	14 ± 4·2	6·2 ± 2·3	4·0 ± 1·5	1·7 ± 0·9	0·80 ± 0·44	0·48 ± 0·26	0·45 ± 0·25	106 ± 31	2·8 ± 0·8
60	200 ± 48	30 ± 7·8	8·1 ± 2·4	2·5 ± 0·75	2·2 ± 1·0	1·7 ± 0·8	1·3 ± 0·7	0·59 ± 0·32	0·40 ± 0·22	71 ± 21	1·9 ± 0·6
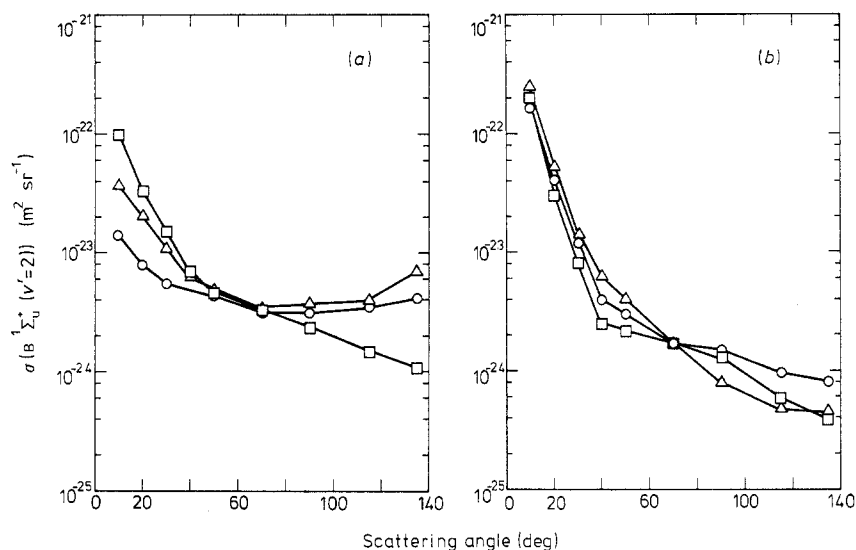
Figure 2. Differential cross sections for the excitation of the $v' = 2$ band of the B $^1\Sigma_u^+$ state of H_2 for (a) electron impact energies of 15 eV (O), 20 eV ($\triangle$) and 30 eV ($\square$) and (b) electron impact energies of 40 eV (O), 50 eV ($\triangle$) and 60 eV ($\square$).

gives values of integral cross sections which are obviously quite high and seem unreasonable. Therefore, these extrapolations were made by continuing the slope between the last two measured data points to 0° and 180° respectively. The areas under these curves were then used to obtain integral cross sections at various energies for the $v' = 2$ band of the B $^1\Sigma_u^+$ state. These results are presented in table 1.

It is evident from figure 1 that at high scattering angles the inelastically scattered signal is very weak and contributes to a large uncertainty in the measurement of the intensity. At lower scattering angles, however, the situation is much better and the results are more accurate. In table 1 the error limits for each cross section are given. In the calculation of these errors, the following sources have been considered: (a) error in the measurements of the intensity of the scattered signal; (b) $\pm15\%$ error in the cross sections σ_{00} for the elastic scattering (Srivastava *et al* 1975a) from H_2; and (c) possible change in the efficiency of the electron energy analyser for detecting elastic- and inelastic-scattering signals. The errors given in table 1 are the square roots of the sums of the squares of individual errors estimated from the above sources. The errors in the integral cross sections contain an additional uncertainty contributed by the extrapolations made to 0° and 180°.

It is known (Lassettre *et al* 1968) that electron impact cross sections for vibrational bands of any electronic state of a molecule are directly proportional to their Frank–Condon factors. For H_2 their calculated values are available (Spindler 1969, Allison and Dalgarno 1970). The data of Allison and Dalgarno agree well, within the experimental errors, with the intensity ratios of spectral features corresponding to $v' = 0$, 1, 2 and 3 vibrational excitations. Their results are also in excellent agreement with the electron-scattering measurements of Geiger (1964) and the photoelectric absorption data of Fabian and Lewis (1974). Therefore, their value for the $v' = 2$ band was used to obtain the total cross section σ_T for exciting the B $^1\Sigma_u^+$ state at each electron impact energy E_0. These results are presented in table 1. The errors in

σ_T have been obtained by direct scaling of the errors for the integral cross sections σ_I.

Acknowledgments

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