J. Phys. B: At. Mol. Opt. Phys. 28 (1995) L393–L397. Printed in the UK

LETTER TO THE EDITOR

Importance of dissociative excitation by slow He^{2+} ions in one-electron capture collisions with H_2

J M Hodgkinson, T K McLaughlin, R W McCullough, J Geddes and H B Gilbody

Department of Pure and Applied Physics, The Queen's University of Belfast, Belfast, UK

Received 17 March 1995

Abstract. Translational energy spectroscopy has been used to study one-electron capture by 0.5–2.0 keV amu^{-1} He^{2+} ions in collision with H_2. The main excited state product channels have been identified and the relative cross sections determined. These measurements provide the first direct evidence of the relative importance of dissociative excitation channels in electron capture (with He^+ formed in the ground state and H atoms mainly in the $n = 2$ states) which *dominate the entire energy range. Non-dissociative electron capture into the* $n = 2$ *and* $n = 3$ states of He^+, which is also observed, increases from 1% of the total electron capture cross section at 0.5 keV amu^{-1} to about 25% at 2 keV amu^{-1}.

The importance of a detailed understanding of heavy-particle collision processes which occur in the edge plasmas of fusion devices is well known (cf Janev 1993). Exothermic electron capture processes with high cross sections at low energies are of particular interest in this context. In the present work we have used translational energy spectroscopy (TES) to study one-electron capture in 0.5–2.0 keV amu^{-1} collisions of He^{2+} ions with H_2 and identify the main excited product channels. The measurements provide the first direct evidence of the dominant role of channels involving dissociative excitation of H_2 at low energies.

In previous work in this laboratory (Graham *et al* 1974), studies of the fragmentation of H_2 by He^{2+} impact indicated that dissociative one-electron capture became important at low keV energies. Measurements in the range 2.2–17.3 keV amu^{-1} showed that total cross sections for H^+ formation (through both electron capture and ionization) below 3 keV amu^{-1} increased with decreasing energy while corresponding cross sections for H_2^+ formation decreased rapidly.

Recent studies by Hoekstra *et al* (1994) in the range 1–25 keV amu^{-1} using photon emission spectroscopy have shown that, above about 5 keV amu^{-1}, He^+ products of one-electron capture are formed primarily in excited states (especially $n = 2$) through the non-dissociative process

$$He^{2+} + H_2 \rightarrow He^+(n \geqslant 2) + H_2^+ {}^2\Sigma_g. \tag{1}$$

However, at energies below about 5 keV amu^{-1}, they have suggested by reference to previous fragmentation studies (Graham *et al* 1974, Afrosimov *et al* 1980) that electron capture takes place primarily through the dissociative channels

$$He^{2+} + H_2 \rightarrow He^+(1s) + H^+ + H(n \geqslant 2). \tag{2}$$

0953-4075/95/120393+05$19.50

The present TES measurements complement previous experimental studies and permit the relative importance of (1) and (2) to be assessed. The measured difference ΔT between the kinetic energy T_1 of the primary He^{2+} ion and the kinetic energy T_2 of the product He^+ ion can be expressed as $\Delta T = (T_2 - T_1) = \Delta E - \Delta K$ where ΔE is the energy defect corresponding to a particular product channel and ΔK is a small target recoil correction. Provided that $\Delta E/T_1 \ll 1$ and the scattering is confined to small angles (McCullough *et al* 1984), $\Delta T \cong \Delta E$. Thus an analysis of the He^+ yields in the observed energy change spectra provided, within the available energy resolution, relative cross sections for product channels characterized by energy defects ΔE.

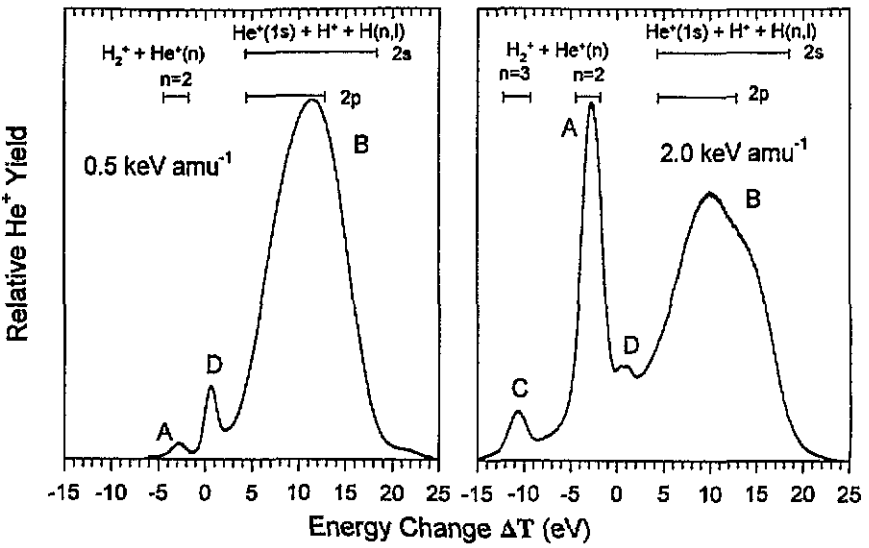

Figure 1. Energy change spectra for one-electron capture by 0.5 and 2 keV amu^{-1} He^{2+} ions in collision with H_2.

The translational energy spectrometer and the measurement procedure have been described in detail in our previous work (see Wilkie *et al* 1986) so that only the essential features need be given here. A momentum analysed primary He^{2+} ion beam, obtained from an electron cyclotron resonance ion source, was focused and decelerated to 120 eV before passage through two hemispherical electrostatic analysers which reduced the energy spread to below 1 eV FWHM. The ion beam was then focused and accelerated to the required energy within the range 0.5–2.0 keV amu^{-1} and passed through hydrogen gas in the target gas cell. The fast forward scattered He^+ products of one-electron capture (within a mean half angle of 0.5°) emerging from the cell were then energy analysed by a third hemispherical electrostatic analyser and counted as pulses by a computer-controlled position-sensitive detector. Great care was taken to ensure that the hydrogen target gas pressure was at all times low enough to ensure single collision conditions.

Figure 1 shows energy change spectra obtained at 0.5 keV amu^{-1} and 2.0 keV amu^{-1}. The energy scale on our measured energy change spectra was calibrated by reference to our previous data for He^{2+}–O_2 collisions (McCullough *et al* 1992). The energy defects ΔE for all possible product channels were obtained by reference to the compilations of Bashkin and Stoner (1987), Kelly (1982) and Sharp (1971). Only those energy defects ΔE showing a strong correlation with the peak yields of He^+ are indicated in these spectra. In the case

Table 1. Collision product channels for one-electron capture by He^{2+} ions in collisions with H_2.

Peak designation	Product channels	ΔE (eV)
A	$He^+(n=2) + H_2^+ {}^2\Sigma_g$	−1.79 to −4.44
B	$He^+(1s) + H^+ + H(2s)$	4.30 to 18.36
	$He^+(1s) + H^+ + H(2p)$	4.40 to 12.73
C	$He^+(n=3) + H_2^+ {}^2\Sigma_g$	−9.38 to −12.35

of the non-dissociative electron capture process (1) leading to He^+ ($n = 2, 3$) channels, the spread in ΔE shown represents the limits of vibrational excitation ($v = 0 \rightarrow \infty$) of the H_2^+ product. In the case of dissociative electron capture process (2), the spread in ΔE shown takes account of the limits associated with Franck–Condon transitions from the $H_2\,{}^1\Sigma_g$ ground state to repulsive states of H_2^+ leading to $H^+ + H(2s)$ and $H^+ + H(2p)$ products. The energy defects and product designations corresponding to the peaks A, B and C in the observed energy change spectra are summarized in table 1.

Peak A at around $\Delta E \cong -3$ eV corresponds to $He^+(n = 2)$ formation in process (1) with H_2^+ formed in the ground state. The broad peak B for ΔE between 5 and 20 eV correlates strongly with the dissociative process (2) leading to H ($n = 2$) excited atoms and He^+ ground-state ions. There may be a small additional contribution to this peak from $He^+(1s) + H^+ + H(n = 3)$ products with ΔE between −2.5 and 12 eV. The minor peak C which is only significant at energies above 1.5 keV amu^{-1} arises from $He^+(n = 3)$ formation in (1).

A curve fitting procedure (PEAKFIT v.3.0 supplied by Jandel Scientific) was used to determine the relative contributions of A, B and C to one-electron capture. Cross sections for these separate channels were then determined by normalization of our total He^+ yields to well established total cross sections σ_{21} for one-electron capture in He^{2+}–H_2 collisions measured previously in this laboratory (Nutt *et al* 1978). These derived cross sections are tabulated in table 2 and shown in figure 2.

Table 2. Measured cross sections for excited product channels in one-electron capture by He^{2+} ions in collision with H_2. Random uncertainties associated with each cross section are shown. In addition all cross sections are subject to an estimated uncertainty of ±11% arising from the normalization procedure.

	Cross sections (10^{-16} cm^2)				
Products	0.5 keV amu^{-1}	1.0 keV amu^{-1}	1.3 keV amu^{-1}	1.5 keV amu^{-1}	2.0 keV amu^{-1}
$He^+(1s) + H^+ + H(2s)$ $He^+(1s) + H^+ + H(2p)$	1.13 ± 0.10	1.44 ± 0.08	1.52 ± 0.09	1.40 ± 0.13	1.39 ± 0.07
$He^+(n=2) + H_2^+ {}^2\Sigma_g$	0.014 ± 0.001	0.107 ± 0.006	0.19 ± 0.01	0.35 ± 0.03	0.48 ± 0.03
$He^+(n=3) + H_2^+ {}^2\Sigma_g$	—	—	—	0.027 ± 0.002	0.075 ± 0.004

It can be seen that the dissociative excitation process (2) becomes increasingly important with decreasing energy with the contribution from peak B increasing from 71% of the total yield at 2.0 keV amu^{-1} to 99% at 0.5 keV amu^{-1}. There is a corresponding decrease in the contribution of the non-dissociative process (1) corresponding to peak A which accounts for 25% of the total at 2.0 keV amu^{-1} and 1% at 0.5 keV amu^{-1}. Peak C, which only becomes significant at 1.5 keV amu^{-1}, comprises 4% of the total signal at 2.0 keV amu^{-1}. In a

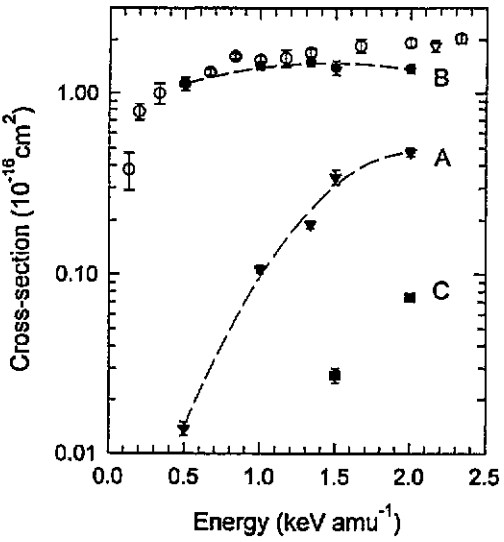

Figure 2. Cross sections for one-electron capture by He^{2+} ions in collision with H_2. Present cross sections for specified product channels: ▼, peak A corresponding to $He^+(n = 2) + H_2^+ {}^2\Sigma_g$; ●, peak B corresponding to $He^+(1s) + H^+ + H(n = 2)$; ■, peak C corresponding to $He^+(n = 3) + H_2^+ {}^2\Sigma_g$. Total cross sections σ_{21} for one-electron capture: ○, Nutt *et al* (1978); ▽, Shah and Gilbody (1978).

subsidiary experiment using a water vapour target we have positively identified peak D at $\Delta E \cong 1$ eV as an impurity product arising from non-dissociative electron capture in traces of water vapour leading to $He^+(n = 2)$. Peak D arises from water vapour in the residual gas at a pressure of 5×10^{-7} Torr. Strong dissociative collision channels in background H_2O have also been recently observed in fast He^+–H_2 collision studies by Beckord *et al* (1994).

It is interesting to note that, if the 2p–1s emission cross sections measured recently by Hoekstra *et al* (1994) for He^{2+}–H_2 collisions are compared with the present cross sections for the dissociative channel (2), they indicate that H(2p) rather than H(2s) formation is dominant in the present energy range. In a previous TES study, Kobayashi *et al* (1984) have also observed the broad peak B in measurements with 0.2–0.5 keV amu^{-1} He^{2+} ions but obtained no evidence of the weak non-dissociative channel involving He^+ formation in excited states. In addition, the TES measurements by Afrosimov *et al* (1980) below 2.5 keV amu^{-1} have shown an increase in $He^+(1s)$ relative to $He^+(n = 2)$ formation.

The present measurements provide the first direct evidence of the dominant contribution of dissociative excitation in electron capture by He^{2+} ions in collisions with H_2 at low keV energies. Cross sections for the main dissociative and non-dissociative product channels have been determined in the range 0.5–2.0 keV amu^{-1}. The dissociative electron capture process involves mainly $He^+(1s) + H^+ + H(n = 2)$ formation. Non-dissociative electron capture, which increases in importance at higher energies, is found to involve mainly $He^+(n = 2, 3) + H_2^+ {}^2\Sigma_g$ formation. The present results indicate an interesting area for detailed theoretical study.

This work is part of a programme supported by a Rolling Grant from the Engineering and Physical Science Research Council. One of us (JMH) is also indebted to the Department of Education, Northern Ireland for the award of a research studentship.

References

Afrosimov V V, Leiko G A and Panov M N 1980 *Sov. Phys. Tech. Phys.* **25** 313
Bashkin S and Stoner J O Jr 1987 *Atomic Energy Levels and Grotrian Diagrams* (Amsterdam: North-Holland)
Beckord K, Becker J, Werner U and Lutz H O 1994 *J. Phys. B: At. Mol. Opt. Phys.* **27** L585
Graham W G, Latimer C J, Browning R and Gilbody H B 1974 *J. Phys. B: At. Mol. Phys.* **7** L405
Hoekstra R, Folkerts H O, Beijers J P M, Morgenstern R and de Heer F J 1994 *J. Phys. B: At. Mol. Opt. Phys.* **27** 2021
Janev R K 1993 *Summary Report of 2nd IAEA Research Coordination Meeting on 'Atomic and Molecular Data for Plasma Edge Studies', International Atomic Energy Agency Report, INDC(NDS)* (Vienna: Austria) p 276
Kelly R L 1982 *ORNL Report* 5492, Oak Ridge National Laboratory, USA
Kobayashi N, Iwai T, Kaneko Y, Kimura M, Matsumoto A, Ohtani S, Okuno K, Takagi S, Tawara H and Tsurubuchi S 1984 *J. Phys. Soc. Japan* **53** 3736
McCullough R W, McLaughlin T K, Koizumi T and Gilbody H B 1992 *J. Phys. B: At. Mol. Opt. Phys.* **25** L193
McCullough R W, Wilkie F G and Gilbody H B 1984 *J. Phys. B: At. Mol. Phys.* **17** 1373
Nutt W L, McCullough R W, Brady K, Shah M B and Gilbody H B 1978 *J. Phys. B: At. Mol. Phys.* **11** 1457
Shah M B and Gilbody H B 1978 *J. Phys. B: At. Mol. Phys.* **11** 121
Sharp T E 1971 *At. Data* **2** 119–69
Wilkie F G, McCullough R W and Gilbody H B 1986 *J. Phys. B: At. Mol. Phys.* **19** 239