J. Phys. B: At. Mol. Opt. Phys. 25 (1992) L127–L130. Printed in the UK

LETTER TO THE EDITOR

Excitation and charge transfer in He^+–H collisions

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Received 9 December 1991

Abstract. We have computed the cross section for excitation of the Balmer alpha line of H, induced by collisions with He^+. The total cross section for charge transfer to He has also been computed. Comparison is made with the corresponding measurements of Donnelly *et al* and Olson *et al*.

Donnelly *et al* (1991) have recently reported measurements of Balmer alpha emission induced by collisions between hydrogen atoms and H^+, He^+ and He^{2+} projectiles. Their results for proton excitation have been compared with new calculations, based on the semiclassical impact parameter method, by Ermolaev (1991). He finds that theory can account for only about a half of the measured value of the cross section near its maximum, at a laboratory energy of about 40 keV.

In the present letter, theoretical data on the production of Balmer alpha radiation by He^+ impact are compared with the corresponding measurements of Donnelly *et al* (1991). Whilst good agreement with the experiment is obtained for the lower impact energies ($10 \leqslant E(^4He^+) \leqslant 40$ keV), the measurements rise above the calculated values of the cross section at higher energies. On the other hand, the total capture cross section is found to agree well with the measurements of Olson *et al* (1977) over the entire energy range.

As in the work of Ermolaev (1991), the semiclassical impact parameter method was employed, with a basis of travelling atomic orbitals on each centre, target and projectile. However, a technical difference is our introduction of Gaussian- (rather than Slater-) type orbitals to describe the atomic states. Gaussian-type orbitals have been used recently by Gramlich *et al* (1989) in their study of charge transfer and ionization in He^{2+}–He collisions; Gaussians have the advantage of enabling all the two-electron integrals over electronic coordinates, including those which involve plane-wave translation factors, to be reduced to recurrence relations and a basic integral which can be rapidly evaluated (Obara and Saika 1986, 1988, Errea *et al* 1979). Of course, more Gaussian- than Slater-type orbitals are required to accurately represent a given atomic state, but this disadvantage is offset by the rapidity of the integral evaluations.

The calculations were performed with a total of 39 atomic states of singlet and 38 states of triplet spin symmetry, representing the He^+–H and He–H^+ systems. For the He^+ ion, six Gaussian orbitals were adopted, with the exponents being the terms of a geometric series in the range (0.03, 20). For H, the range of the exponents of the eight Gaussians was (0.004, 8), and for He seven Gaussians (0.008, 50). The endpoints of the geometric series were initially chosen by reference to the work of Gramlich *et al* (1989) but subsequently varied to optimize the computed eigenenergies. The atomic

0953-4075/92/050127+04$04.50

states and the corresponding values of their measured and calculated energies are listed in table 1. The $n = 4$ states of H are not well represented by the chosen Gaussian basis and should be regarded as pseudostates enabling a correction to be made for the cascade (to $n = 3$) contribution from higher energy states of hydrogen. In practice, the cascade correction was found to be small (cf Ermolaev 1991), never more than 10% of the direct contribution, given by

$$\sigma(\text{direct}) = \sigma(3\text{s}) + 0.12\sigma(3\text{p}) + \sigma(3\text{d})$$

where the cross sections on the right-hand side are for direct excitation. The numerical results are given in table 2.

Table 1. Measured (cf Gramlich *et al* 1989) and calculated (this work) energies of the states of the He^+-H and He-H^+ systems.

	Energy (Hartree)	
State	Calculated	Measured
H 1s	−0.4991	−0.5000
2s	−0.1248	−0.1250
$2p_0, \pm 1$	−0.1249	−0.1250
3s	−0.0551	−0.0555
$3p_{0\pm 1}$	−0.0554	−0.0555
$3d_{0,\pm 1,\pm 2}$	−0.0555	−0.0555
4s	−0.0183	−0.03125
$4p_{0,\pm 1}$	−0.0289	−0.03125
$4d_{0,\pm 1,\pm 2}$	−0.0310	−0.03125
He $1s^2\,{}^1S$	−2.874	−2.904
$1s2s\,{}^3S$	−2.169	−2.175
$1s2s\,{}^1S$	−2.140	−2.146
$1s2p_{0,\pm 1}\,{}^3P$	−2.128	−2.133
$1s2p_{0,\pm 1}\,{}^1P$	−2.118	−2.124
$1s3s\,{}^3S$	−2.064	−2.069
$1s3s\,{}^1S$	−2.055	−2.061
$1s3p_{0,\pm 1}\,{}^3P$	−2.053	−2.058
$1s3p_{0,\pm 1}\,{}^1P$	−2.050	−2.055
He 1s	−1.992	−2.000
2s	−0.498	−0.500

Table 2. Cross sections (in units of 10^{-18} cm^2) for direct excitation of the Balmer α line, together with the cascade correction and the corrected values. E($^4He^+$) is the impact energy of the $^4He^+$ projectile on the H target.

E($^4He^+$) (keV)	σ (direct)	σ (cascade)	σ (corrected)
10	2.08	0.20	2.28
15	5.87	0.09	5.96
20	8.83	0.20	9.03
40	6.91	0.35	7.26
80	6.57	0.50	7.07
120	5.61	0.40	6.01
200	6.91	0.46	7.37
400	6.45	0.55	7.00

The calculations were performed on the Meiko Computing Surface in the Physics Department of Durham University. The FORTRAN code was run within the FORTNET Occam harness of Allan *et al* (1990), which enables data farming to be carried out. The computation time was typically 140 h per energy, using a domain of 9 Inmos T-800 transputers.

In figure 1, the computed values of the cross sections for production of Balmer alpha radiation by He^+ impact are compared with the measurements of Donnelly *et al* (1991); the theoretical results have been corrected for cascade contributions. As may be seen from the figure, the calculations reproduce the measurements quite well for $E(^4He^+) \leqslant 40$ kev, beyond which there is an increase in the experimental cross section which is not seen in theory. Indeed, the measurements suggest the onset of an additional process which contributes to the production of Balmer alpha radiation above about 40 keV. What this process might be remains unclear. One possibility is that the ionization channels, neglected in the present calculations, might indirectly affect the excitation cross sections at the higher energies. On the other hand, structure similar to that observed for He^+-H is not seen in the measurements for H^+-H. Further experimental and theoretical work is required to clarify this issue.

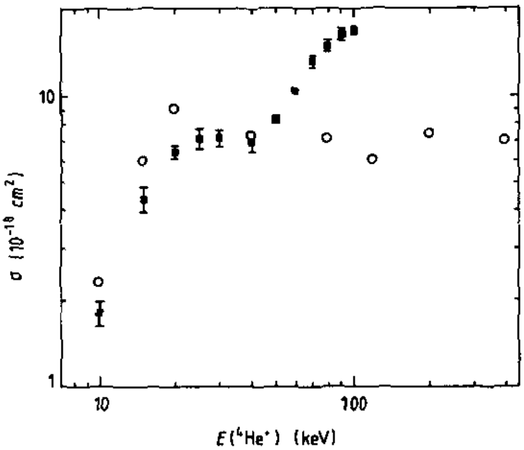

Figure 1. Measured (full squares with errors bars, Donnelly *et al* (1991)) and calculated (after correction for cascade, open circles, this work) cross sections for excitation of the H Balmer α line by $^4He^+$ impact.

Donnelly *et al* (1991) interpret the cross section above 40 keV as arising from direct excitation of $H(n=3)$ and suggest that, *below* 40 keV, the shoulder on the measured curve arises owing to coupling with charge transfer to excited states of He which are energetically close to $He^+(1s)+H(n=3)$. As may be seen from table 1, such a state is $He(1s3p\,^1P)$. This state was included in our basis set and, as noted above, the computed values of the Balmer alpha cross section below 40 keV agree with experiment. We believe rather that it is *above* 40 keV where an additional process may be intervening, for which, as yet, allowance has not been made in the calculations.

In figure 2 are presented the measured (Olson *et al* 1977) and computed values of the cross section for the process

$$H(1s)+{}^3He^+(1s)\rightarrow H^+ + {}^3He.$$

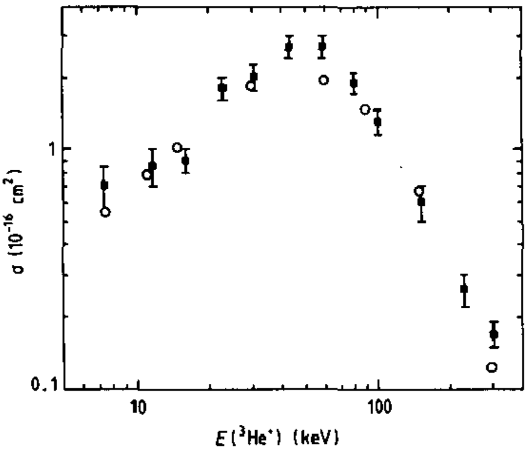

Figure 2. Measured (full squares with error bars, Olson *et al* (1977)) and calculated (open circles, this work) total charge transfer cross section for $^3He^+$–H collisions.

In this case, there is good agreement between theory and experiment over the entire energy range. Although this agreement does not guarantee the reliability of the Balmer alpha cross section, it is reassuring that our approach accounts correctly for the dominant process (charge transfer) in the intermediate energy range.

This work has been supported by the SERC, through the provision of a research studentship to David Jackson and part-funding of the Meiko Computing Surface. We have benefited from discussions with Dr Ian Cooper and assistance with the use of the Meiko Computing Surface from Dr Lydia Heck.

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