

Absolute differential and integral cross sections for charge transfer of keV O^+ ions with CO_2

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Abstract. We report measurements of the absolute differential cross sections for charge-transfer scattering of 0.5, 0.85, 1.5, 2.8 and 5 keV O^+ ions by CO_2 at scattering angles between 0.04° and 2.9° in the laboratory frame. Cross sections for both $O^+(^4S)$ ground-state and $O^+(^2D, ^2P)$ metastable ions are presented. The angular dependence of the differential cross sections is similar for both ground-state and metastable ions but the ground-state integral cross section is greater than that for metastable ions over most of the energy range considered.

1. Introduction

Charge transfer reactions of O^+ ions are important in many diverse areas of science and technology from plasma devices to planetary atmospheres (Stebbing *et al* 1966, Flesch and Ng 1991) and consequently considerable effort has been expended in their study. The situation is complicated, however, by the fact that oxygen ions are typically present in both the ground 4S state and in the long-lived excited metastable 2D and 2P states. In collisions with atoms and molecules the behaviour of the O^+ ions in these various states is generally dissimilar, occasionally markedly so. For most of the targets that have been studied to date it has been found that, in the energy range considered here, the charge-transfer cross section for O^+ ground-state ions is smaller than that for O^+ metastable ions. In the case of O^+-N_2 , for instance, differences of greater than an order of magnitude were observed (Lindsay *et al* 1998). However, in the only previous study of O^+ with a CO_2 target, in which both ground-state and metastable species were investigated (Moran and Wilcox 1978), the opposite was found to be true; for projectile energies in the vicinity of 1 keV the ground-state O^+ cross section was found to be approximately twice as great as that for the metastable ion. These observations are consistent with energy defect considerations which favour the reaction of metastable O^+ ions over ground-state O^+ ions in many of the systems investigated previously, whereas in the case of O^+-CO_2 the opposite is true (Moran and Wilcox 1978). Until a very short time ago there had also been no work on the angular differential cross sections (DCSs) for O^+ charge transfer. This study has been performed both to remedy this situation and to provide additional data on the relative magnitudes of the ground-state and metastable-state O^+-CO_2 cross sections.

A variety of experimental strategies have been employed to measure state-selected O^+ charge-transfer cross sections. It is possible, for example, to obtain a beam of pure ground-state O^+ ions by utilizing an electron bombardment ion source in which the electron energy is

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held below the threshold for excited ion production. Analogous procedures are not, however, readily available for the production of pure $O^+(^2D)$ and $O^+(^2P)$ beams and consequently laboratory studies of metastable O^+ reactions are usually conducted with a beam initially comprised of both ground-state and excited-state ions. Some variation of the attenuation curve technique (Stebbing *et al* 1966, Turner *et al* 1968) has then generally been employed to extract the individual cross sections[†]. This technique is itself based on the fact that, for certain targets, the excited ions and the ground-state ions have very different charge-transfer cross sections. In passing through such a target the different components of a mixed state beam are therefore attenuated at different rates. This effect has been exploited in two ways. For target gases for which the ground- and excited-state cross sections are markedly dissimilar the relative abundances of the different components and their individual cross sections may be determined directly from the attenuation curves (Stebbing *et al* 1966, Nutt *et al* 1979, Xu *et al* 1990). In other situations an appropriately selected gas may be used to ‘filter’ out one component from a mixed state beam (Lindsay *et al* 1998). The transmitted beam is then predominantly comprised of the other component whose cross section may be determined.

Almost all studies on state-selected O^+ ions, in which metastable cross sections have been determined, have involved some variant of the attenuation curve technique, although it must be emphasized that this technique is not as precise as one would like. Its use to derive total cross sections is experimentally challenging due to elastic scattering issues, and moreover the simple analysis of the attenuation curves generally employed neglects second-order effects such as stripping of the fast neutrals (McDaniel *et al* 1993). It has also not been possible to distinguish between the two metastable species using this technique alone and the metastable cross sections reported therefore pertain to an indeterminate mix of $O^+(^2D)$ and $O^+(^2P)$. However, despite its limitations, and in the absence of superior methods, the continued use of the attenuation curve technique appears warranted. In the present study it has been used solely to determine the fraction of excited-state O^+ ions in the beam, rather than the cross sections themselves, and it is estimated that any error resulting from its use in this context will be significantly smaller than the quoted uncertainties in the data presented here.

2. Apparatus and experimental method

The apparatus and the experimental method have both been described in detail previously (Lindsay *et al* 1998). The apparatus is shown in figure 1. CO is admitted to a magnetically confined plasma ion source. Ions are extracted from the source through a small aperture, accelerated, and focused to form a beam of the desired energy. Two confocal 60° sector magnets are used to select ions of the desired mass-to-charge ratio. Ions passing through a pair of laser-drilled apertures, separated by 23 cm, form a beam with an angular divergence of approximately 0.03° . The first aperture, 100 μm in diameter, forms the exit of the filter cell. The second aperture, 20 μm in diameter, forms the entrance to the target cell whose length is approximately 1 mm. A 200 μm aperture forms the exit of the target cell. A position-sensitive detector (PSD) located 26 cm beyond the target cell serves to measure the flux of ions passing through the target cell and to measure the flux and positions of impact of product neutral O atoms. A pair of deflection plates located between the target cell and the PSD is used to deflect the ion beam when required.

In order to measure the differential charge-transfer cross section, CO_2 is admitted to the target cell and the angles of scatter of the neutral O atoms, formed by charge transfer of

[†] A notable exception is the series of experiments performed by Ng and co-workers, e.g. Li *et al* (1997).

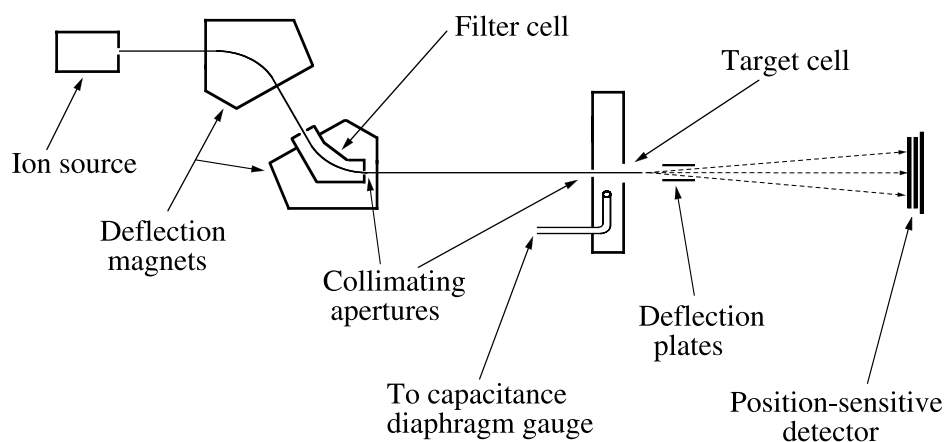


Figure 1. Schematic of the apparatus.

the primary O^+ ions, are determined from their positions of impact on the PSD. Unscattered primary O^+ ions are normally deflected from the PSD but are allowed to impact the PSD periodically to assess the primary beam flux. These measurements, together with the target number density and target length are sufficient to determine the DCS. The O^+ beam, as it emerges from the ion source, comprises both ground-state and metastable-state ions. Cross sections for both components of the ion beam are obtained by utilizing the fact that $O^+(^4S)$ ground-state ions have a much smaller charge-transfer cross section with N_2 than $O^+(^2D, ^2P)$ metastable ions. During the measurement of the ground-state cross section the filter cell is filled with several mtorr of N_2 . The emerging O^+ beam then consists essentially of only ground-state ions as practically all of the incident $O^+(^2D, ^2P)$ ions are converted to neutrals, which because of the apparatus geometry do not enter the target cell (Lindsay *et al* 1998). The $O^+(^2D, ^2P)$ cross section is determined by evacuating the filter cell, measuring the effective cross section for the mixed composition beam, determining the fraction of ions in the ground state, and subtracting the contribution these ground-state ions have made to the total scattering signal. The effective cross section measurement and two fraction measurements are generally made within a period of less than 1 h. The fraction of ions in the ground and excited states is measured using a modified version of the attenuation technique originally developed by Stebbings *et al* (1966). As noted in a previous publication (Lindsay *et al* 1998) only two components are identifiable from these attenuation curves, a ground-state component and a metastable excited-state component.

3. Results and discussion

The DCSs for charge transfer of $O^+(^4S)$ and $O^+(^2D, ^2P)$ with CO_2 are shown in figure 2 and selected values are tabulated in tables 1 and 2. Besides the statistical uncertainties shown there is an additional systematic uncertainty of approximately 12% in the absolute magnitude of the DCSs. The angular uncertainties arise from the finite primary beam size and the angular resolution used for analysis. All of the cross sections are very forward peaked, as would be expected for near-resonant processes. The DCSs for ground-state and metastable-state ions are almost identical except at the lowest projectile energy where the metastable cross section is slightly less forward peaked.

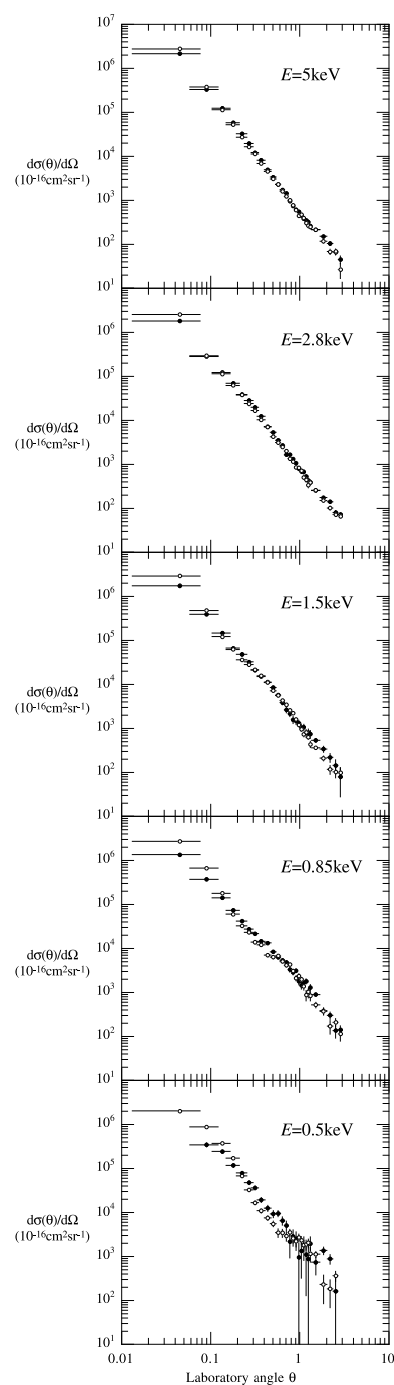


Figure 2. Absolute differential cross sections for charge-transfer scattering of $\text{O}^+(^4\text{S})$ by CO_2 (open circles) and $\text{O}^+(^2\text{D}, ^2\text{P})$ by CO_2 (full circles) at the projectile energies indicated.

Table 1. Laboratory frame differential $O^+(^4S)$ – CO_2 charge-transfer cross sections, where E is the projectile energy and the numbers in square brackets represent powers of ten.

Laboratory angle θ (deg)	$d\sigma(\theta)/d\Omega$ (10^{-16} cm 2 sr $^{-1}$)				
	$E = 0.5$ keV	$E = 0.85$ keV	$E = 1.5$ keV	$E = 2.8$ keV	$E = 5$ keV
0.04 ± 0.03	$2.01 \pm 0.04[6]$	$2.72 \pm 0.04[6]$	$2.90 \pm 0.02[6]$	$2.52 \pm 0.02[6]$	$2.73 \pm 0.02[6]$
0.09 ± 0.03	$8.71 \pm 0.20[5]$	$6.63 \pm 0.15[5]$	$4.75 \pm 0.07[5]$	$2.91 \pm 0.05[5]$	$3.75 \pm 0.04[5]$
0.18 ± 0.03	$1.70 \pm 0.06[5]$	$5.98 \pm 0.32[4]$	$6.18 \pm 0.18[4]$	$6.16 \pm 0.16[4]$	$5.21 \pm 0.11[4]$
0.37 ± 0.04	$1.09 \pm 0.13[4]$	$1.20 \pm 0.09[4]$	$1.56 \pm 0.05[4]$	$1.03 \pm 0.04[4]$	$6.88 \pm 0.23[3]$
0.71 ± 0.04	$2.89 \pm 0.69[3]$	$4.11 \pm 0.43[3]$	$3.45 \pm 0.17[3]$	$2.00 \pm 0.12[3]$	$1.22 \pm 0.07[3]$
1.52 ± 0.17	$1.12 \pm 0.19[3]$	$5.21 \pm 0.81[2]$	$3.61 \pm 0.30[2]$	$2.56 \pm 0.17[2]$	$2.14 \pm 0.11[2]$
2.87 ± 0.17	—	$1.14 \pm 0.37[2]$	$9.8 \pm 2.8[1]$	$6.64 \pm 0.61[1]$	$2.7 \pm 1.0[1]$

Table 2. Laboratory frame differential $O^+(^2D, ^2P)$ – CO_2 charge-transfer cross sections, where E is the projectile energy and the numbers in square brackets represent powers of ten.

Laboratory angle θ (deg)	$d\sigma(\theta)/d\Omega$ (10^{-16} cm 2 sr $^{-1}$)				
	$E = 0.5$ keV	$E = 0.85$ keV	$E = 1.5$ keV	$E = 2.8$ keV	$E = 5$ keV
0.04 ± 0.03	—	$1.34 \pm 0.05[6]$	$1.73 \pm 0.05[6]$	$1.80 \pm 0.02[6]$	$2.13 \pm 0.02[6]$
0.09 ± 0.03	$3.44 \pm 0.41[5]$	$3.70 \pm 0.16[5]$	$3.92 \pm 0.15[5]$	$2.82 \pm 0.06[5]$	$3.30 \pm 0.04[5]$
0.18 ± 0.03	$1.17 \pm 0.13[5]$	$7.34 \pm 0.37[4]$	$6.62 \pm 0.41[4]$	$6.92 \pm 0.19[4]$	$5.81 \pm 0.12[4]$
0.37 ± 0.04	$1.92 \pm 0.26[4]$	$1.44 \pm 0.10[4]$	$1.51 \pm 0.11[4]$	$1.23 \pm 0.05[4]$	$8.09 \pm 0.26[3]$
0.71 ± 0.04	$5.0 \pm 1.4[3]$	$4.80 \pm 0.47[3]$	$2.62 \pm 0.39[3]$	$1.65 \pm 0.14[3]$	$1.43 \pm 0.08[3]$
1.52 ± 0.17	$7.4 \pm 3.6[2]$	$8.89 \pm 0.82[2]$	$5.33 \pm 0.60[2]$	$2.53 \pm 0.20[2]$	$2.15 \pm 0.12[2]$
2.87 ± 0.17	—	$1.40 \pm 0.36[2]$	$7.9 \pm 5.2[1]$	$7.27 \pm 0.74[1]$	$4.5 \pm 1.0[1]$

From inspection of the differential cross sections shown in figure 2 it is possible to infer the extent to which neutrals are scattered at angles sufficiently large to avoid impacting the PSD. It is estimated that the fraction of scattered neutrals which do not impact the PSD is negligibly small for 5 keV projectiles ($<1\%$) but may be as large as 25% at the lowest projectile energy studied here. With this in mind, it is possible to compare the present integral cross sections, which necessarily represent a lower limit to the total cross sections, with previously measured total cross sections. This comparison is shown for $O^+(^4S)$ in figure 3. It should be noted that the cross sections presented here and those of Moran and Wilcox (1978) are for production of fast neutral O charge-transfer products, while those of Rutherford and Vroom (1976) and Flesch and Ng (1991) are for production of slow CO_2^+ charge-transfer product ions. These cross sections should, however, be equivalent as both Rutherford and Vroom (1976) and Flesch and Ng (1991) have shown that the only slow product ion of any significance produced at the energies studied here is CO_2^+ . The figure reveals that the present ground-state cross section and the earlier ground-state data of Moran and Wilcox (1978) are not in good agreement with one another since based on the shapes of the differential cross sections shown in figure 2 it seems improbable that the difference between them can be wholly accounted for by the fact that the present cross sections are integral rather than total. They are, however, both consistent with the data of Rutherford and Vroom (1976) and with the relatively recent data of Flesch and Ng (1991).

The present data (table 3) show that, over most of the energy range considered here, the ground-state O^+ cross section is indeed greater than that for metastable O^+ , confirming this aspect of the earlier Moran and Wilcox (1978) study. However, below approximately 2 keV the magnitude of the difference between the present cross sections is smaller than reported

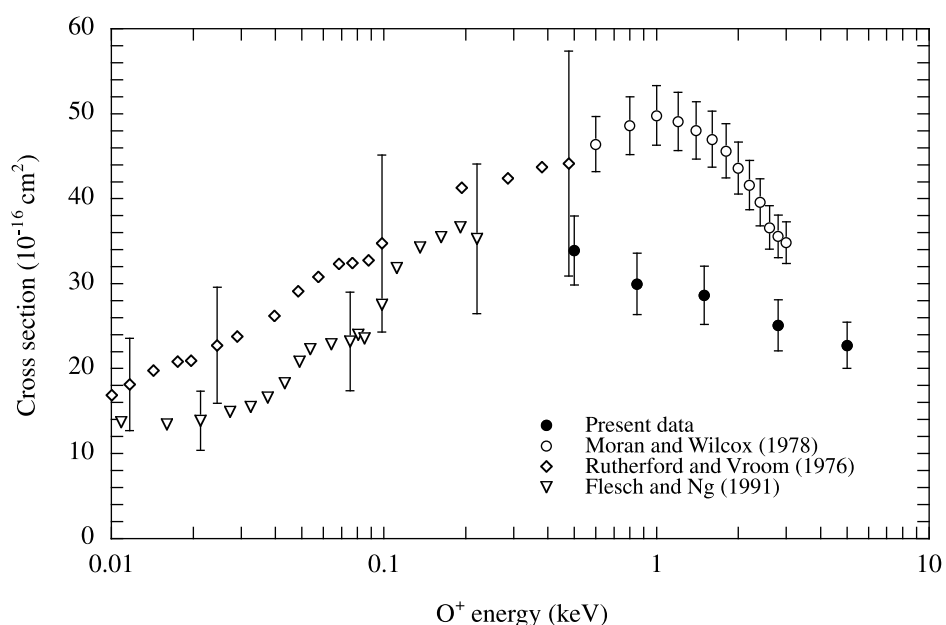


Figure 3. Present absolute integral $O^+(^4S)$ – CO_2 charge-transfer cross sections compared to previously measured total cross sections.

Table 3. Absolute integral O^+ – CO_2 charge-transfer cross sections. The angular range for the integral cross sections is 0° – 3.4° .

Projectile energy (keV)	Cross section (10^{-16} cm^2)	
	$O^+(^4S)$	$O^+(^2D, ^2P)$
0.50	33.9 ± 4.1	19.6 ± 2.4
0.85	30.0 ± 3.6	22.0 ± 2.6
1.5	28.6 ± 3.4	22.1 ± 2.6
2.8	25.1 ± 3.0	23.1 ± 2.8
5.0	22.7 ± 2.7	22.5 ± 2.7

previously. The present metastable cross section together with the data of Moran and Wilcox (1978) is shown in figure 4. As noted earlier, the present metastable data correspond to some unknown mix of $O^+(^2D)$ and $O^+(^2P)$. The Moran and Wilcox (1978) data are reported to pertain to $O^+(^2D)$ ions alone. However, it has been shown that the use by these workers of O_2 in their ion source would almost certainly have produced an O^+ beam consisting of both $O^+(^2D)$ and $O^+(^2P)$ ions (Hamden and Brenton 1989). The metastable cross sections reported by Moran and Wilcox (1978) (figure 4) are in agreement with those presented here at the lowest energies studied but the agreement becomes increasingly poor as the projectile energy increases. At 3 keV the Moran and Wilcox (1978) data are approximately 50% higher than those presented here. The origin of the disagreement between the two sets of data is unclear although it is probable that the excited-state contributions of 2D and 2P ions were different in the two experiments. Furthermore, it should be noted that, whereas in the present study the fractions of excited- and ground-state ions were determined directly, in the work of Moran and

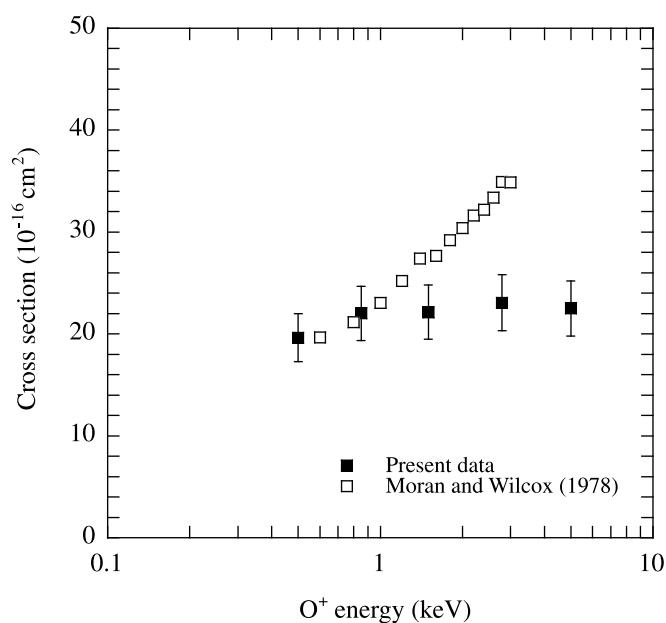


Figure 4. Present absolute $O^+(^2D, ^2P)-CO_2$ integral charge-transfer cross sections compared to the $O^+(^2D)-CO_2$ total cross sections of Moran and Wilcox (1978). The uncertainty in the Moran and Wilcox (1978) data is quoted as $\pm 7\%$ but may be greater because of assumptions made by these workers with regard to their beam composition.

Wilcox (1978) the beam composition was assumed to be the same as that observed by Turner *et al* (1968).

4. Conclusion

The absolute differential cross sections for charge-transfer scattering of 0.5, 0.85, 1.5, 2.8 and 5 keV $O^+(^4S)$ and $O^+(^2D, ^2P)$ by CO_2 at scattering angles between 0.04° and 2.9° in the laboratory frame have been determined. The angular dependence of the differential cross sections is similar for both ground-state and metastable-state ions. The ground-state cross section is greater than that for the metastable state over most of the energy range considered but the observed difference between the two is smaller than previously reported. The integral cross sections reported here are consistent with two of the three prior studies.

Acknowledgments

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References

- Flesch G D and Ng C Y 1991 *J. Geophys. Res.* **96** 21 403–5
- Hamden M and Brenton A G 1989 *J. Phys. B: At. Mol. Opt. Phys.* **22** 2289–95
- Li X, Huang Y-L, Flesch G D and Ng C Y 1997 *J. Chem. Phys.* **106** 564–71
- Lindsay B G, Merrill R L, Straub H C, Smith K A and Stebbings R F 1998 *Phys. Rev. A* **57** 331–7

- McDaniel E W, Mitchell J B A and Rudd M E 1993 *Atomic Collisions: Heavy Particle Projectiles* (New York: Wiley)
- Moran T F and Wilcox J B 1978 *J. Chem. Phys.* **69** 1397–405
- Nutt W L, McCullough R W and Gilbody H B 1979 *J. Phys. B: At. Mol. Phys.* **12** L157–61
- Rutherford J A and Vroom D A 1976 *J. Chem. Phys.* **64** 3057–59
- Stebbins R F, Turner B R and Rutherford J A 1966 *J. Geophys. Res.* **71** 771–84
- Turner B R, Rutherford J A and Compton D M J 1968 *J. Chem. Phys.* **48** 1602–8
- Xu Y, Thomas E W and Moran T F 1990 *J. Phys. B: At. Mol. Opt. Phys.* **23** 1235–43