

Recombination of O^{2+} ions by electron capture from atomic hydrogen in photo-ionized nebulae

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Received 22 February 1994 / Accepted 20 January 1995

Abstract. Detailed calculations are presented of cross sections and rate coefficients at thermal energies for electron capture by 3P ground state O^{2+} ions from atomic hydrogen. The rate coefficient remains practically constant, between 1.1 and $1.2 \cdot 10^{-9} \text{ cm}^3 \text{ s}^{-1}$ in the temperature range from 200 to 20 000 K. The rate coefficient for electron capture by O^{2+} to ions in the metastable 1D or 1S states is negligible at temperatures less than 10^6 K.

Key words: atomic processes – ISM: abundances – H II regions – planetary nebulae

1. Introduction

Charge transfer (or electron capture) reactions play an important role in astrophysical photoionized nebulae (Aldrovandi et al. 1973; Gould 1978; Péquignot et al. 1978, 1991; Dalgarno et al. 1978). Although they have little effect on the overall ionization balance of H^+ , He^+ , He^{2+} ions, they do control the ionization balance of many complex ions and so have a profound influence on the observed emission spectra. Péquignot et al. (1978) were the first to undertake a detailed study of the phenomenon in a specific object. They included charge transfer reactions of C^{3+} , S^{3+} , N^{2+} , O^{2+} , Ne^{2+} ions with atomic hydrogen in a theoretical model of the planetary nebula NGC 7027 whose emission lines had been extensively observed (Kaler et al. 1976; Condal et al. 1981; Giddings 1983; Aller et al. 1988; Keyes et al. 1990). Prior to their work, it had been assumed that ions recombined only by direct radiative or by dielectronic recombination. Their results confirmed that the residual neutral atomic hydrogen density can be sufficiently high for the charge exchange rate to exceed the direct radiative and dielectronic recombination rates. Another interesting consequence is related to the high state selectivity of the charge exchange process, which tends to populate just

a small number of specific excited states. This leads to a considerable enhancement of certain emission features. Subsequent studies by Péquignot et al. (1980a,b) confirm the large influence of charge transfer as a recombination mechanism.

The specific nature of the charge exchange process is such that certain objects like planetary nebulae, with their rich emission lines spectra (Shields et al. 1983), can often be considered as natural “laboratories” to determine theoretical cross sections and rate coefficients at thermal energies. It is a windfall for theorists because it is quite difficult to attain astrophysical energies in laboratory experiments. For although, experimental measurements at higher energies can and do give valuable information, their extrapolation to lower energies can be misleading. Astrophysical charge transfer reactions which are well understood involve O^{3+} (Clegg et al. 1985; Gargaud et al. 1989), Ne^{2+} (Forster et al. 1991), C^{3+} (Opradolce et al. 1988), N^{2+} (Herrero et al. 1994), N^{3+} (Gargaud & McCarroll 1985), Si^{2+} (Gargaud et al. 1982). See also reviews by Péquignot (1988) and McCarroll (1988) for a more global aspects of the charge transfer in astrophysical plasmas.

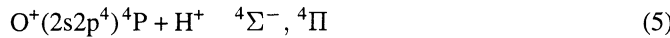
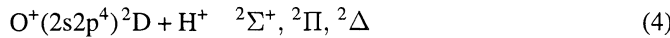
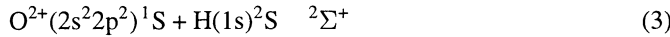
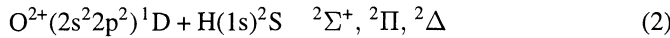
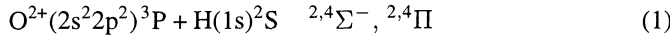
One key charge transfer reaction which is still poorly understood is that between doubly charged oxygen ion O^{2+} and atomic H. The reasons are two-fold. Firstly, the energetically favoured reaction occurs via capture to the $(2s2p^4)^4P$ state of O^+ , which involves the simultaneous capture into a 2p orbital and the excitation of a 2s orbital. Secondly, the open-shell character of the O^{2+} ion implies a multi-channel reaction. The reaction of O^{2+} with H was first considered by Butler et al. 1979 and Butler et al. 1980a using a Landau Zener type model. Subsequently they carried out a series of quantum calculations (Butler et al. 1980b and Butler et al. 1984). The precision of these earlier calculations is a little uncertain, since the molecular data on which they were based does not reproduce well the experimental charge transfer data at higher collision energies. New calculations by Honvault et al. (1994) of the adiabatic energies of the OH^{2+} molecular ion and the corresponding non-adiabatic couplings appear to be more satisfactory. Their calculations of the charge transfer cross

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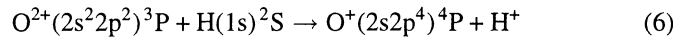
sections in the 100 eV energy range are in much better agreement with the experimental energy gain spectra of McLaughlin et al. (1990) than are the calculations of Heil et al. (1983). There is also some evidence from the astrophysical data that the rate coefficients of Butler et al. (1980b) are too low to explain either the intensity of the observed O^{2+} line at 372.7 nm or the ionization equilibria in the planetary nebula NGC 7027 (Gruenwald et al. 1989). Similarly Petitjean et al. (1990) in their study of old nova shell DQ Herculis 1934 confirm the need for a reliable rate coefficient at low temperatures (around 500 K). First of all, we present below the molecular structure calculation.

2. Theory

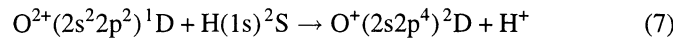
The molecular structure calculation of the OH^{2+} system using an *ab-initio* method has been described in detail by Honvault et al. (1994). As a consequence we will only recall here the essential features of the capture process for which the possible reaction channels (and the adiabatic states to which they are correlated) are designated as follows:



In the typical astrophysical plasmas of concern the metastable 1S and 1D states of O^{2+} ions should be weakly populated (compared with the ground state 3P). We shall therefore limit this study to the reaction with O^{2+} in the 3P ground state. From the potential energy curves calculated by Honvault et al. is clear that of the 4 adiabatic states correlated to channel (1) only the $^4\Sigma^-$ and $^4\Pi$ adiabatic states are subject to avoided crossings. It follows that charge exchange will take place principally via the reaction



Nevertheless, in order to test the contribution of the metastable states to the charge exchange reaction, we shall also include in Sect. 3 some results concerning the reaction:



In Fig. 1 we present the adiabatic energy curves relative to reactions (6). These have been calculated by means of a configuration interaction method based on the CIPSI algorithm (Huron et al. 1973). For states of $^4\Sigma^-$ symmetry we observe only one avoided crossing around $R_x = 3.5a_0$ whereas for states of $^4\Pi$ symmetry there are two avoided crossings around $R_x = 2.5$ and $4.5a_0$. The position R_x of these avoided crossings and the corresponding minimum energy separation ΔE_x are crucial parameters for a good description of the collision dynamics. In Table 1 we compare these parameters with the asymptotic values of Butler et al. (1980a): we see that in spite of the rather

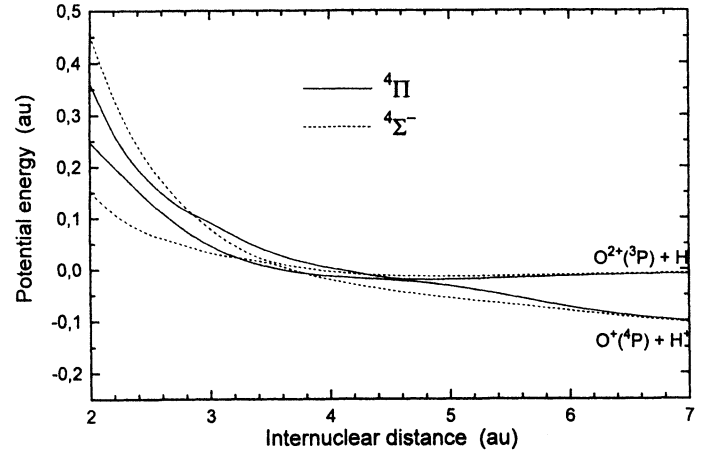


Fig. 1. Adiabatic potential energy curves of the $^4\Sigma^-$ and $^4\Pi$ states of the OH^{2+} molecular ion. Curve A designates the state dissociating to $O^{2+}(^3P) + H(^2S)$, curve B the state dissociating to $O^+(^4P) + H^+$. The dashed curves (---) designate states of $^4\Sigma^-$ symmetry, the solid curves (—) states of $^4\Pi$ symmetry

Table 1. Crossing radii $R_x(a_0)$ and minimum energy separation $\Delta E_x(\text{eV})$ concerning the $^4\Sigma^-$ and $^4\Pi$ states of the OH^{2+} molecular ion. The results are compared with those of Butler et al.

State	Present work		Butler et al.	
	$R_x(a_0)$	$\Delta E(\text{eV})$	$R_x(a_0)$	$\Delta E(\text{eV})$
$^4\Sigma^-$	3.5	0.111	3.7	1.05
$^4\Pi$	2.5	1.063	2.5	2.56
$^4\Pi$	4.5	0.102	4.8	0.38

good agreement on the pseudo-crossing positions, the minimum energy separations are quite different. In all cases our pseudo-crossings tend to be more diabatic, our values of ΔE_x being much sharper.

The results of Table 1 explain why our non-adiabatic couplings should be greater than those of Heil et al. (Fig. 2). For the outer $^4\Pi$ crossing at $R_x = 4.5a_0$ our radial coupling attains a maximum of 2.16 a.u. compared with 1.6 u.a. obtained by Heil et al. For the $^4\Sigma^-$ crossing at $R_x = 3.5a_0$, the difference is more striking: our radial coupling maximum is a factor of 8 greater than the value of Heil et al. We may therefore expect our capture cross sections and rate coefficients to differ significantly from those of Heil et al., since the reaction rates depend strongly on these curve crossings parameters.

The semi-classical method for the collision dynamics calculation used by Honvault et al. in the keV energy range, is not satisfactory in the thermal-eV range (10^{-2} to 10 eV), where orbiting and tunnelling effects appear. It is therefore more appropriate to use a quantum mechanical method. We have used the method described by Gargaud et al. 1981, 1987.

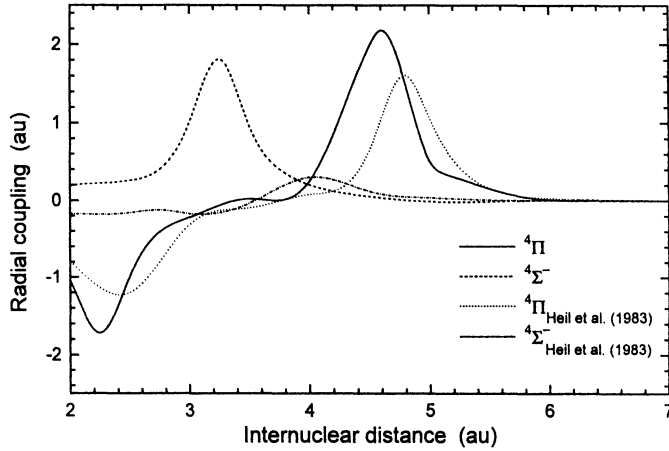


Fig. 2. Non-adiabatic radial coupling matrix elements of the OH^{2+} molecular ion. The dashed curve (---) refers to the matrix element connecting the $4\Sigma^-$ states, the solid curve (—) to the matrix element connecting the 4Π states

Table 2. Charge transfer cross sections (10^{-16} cm^2) in collisions of $O^{2+}(^3P)$ and $O^{2+}(^1D)$ ions with atomic H. The energy (eV) is the relative kinetic Energy

$E(\text{eV})$	$Q(^3P)$	$Q(^1D)$	$Q(\text{Heil } ^3P)$
0.00027	214.98		
0.0135	96.96		
0.0027	87.03		
0.0136	50.55		
0.027	55.86	0.005	
0.136	20.39	0.013	
0.27			10.2
0.272	13.77	0.010	
1.36	6.04	0.011	
1.51			7.66
2.72	5.41	0.013	
3.9			7.80

3. Results

We report in Table 2 the $Q(^3P)$ and $Q(^1D)$ (respectively the cross sections for charge transfer related to reactions 6 and 7) as a function of relative kinetic energy. The metastable 1S state channel (3) has a negligible cross section.

At very low energies, charge exchange occurs only by reaction (6) from ground state 3P ions. Charge exchange by reaction (7) from 1D metastable ions is unimportant for energies less than about 50 eV. This result is consistent with the semi-classical calculations of Honvault et al. at higher energies. The only other available values of cross sections are those of Heil et al. for the reaction (6). At energies exceeding 20 eV the calculated cross sections of Heil et al. are higher than ours by about 30%. On the other hand, in the low energy range (less than 10 eV) the results of Heil et al. are smaller than ours. These differences can be

Table 3. Charge transfer rate coefficient k^3P ($10^{-9} \text{ cm}^3 \text{ s}^{-1}$) between ground state $O^{2+}(^3P)$ ions and atomic H as a function of temperature (K). These are compared with the results of Butler et al.

$T(\text{K})$	k^3P	k^3P (Butler)
100	0.86	—
200	1.07	—
500	1.18	—
1 000	1.15	—
2 000	1.08	—
5 000	1.02	0.60
10 000	1.07	0.77
20 000	1.22	1.03
30 000	1.35	1.26
50 000	1.57	1.62
100 000	1.98	—

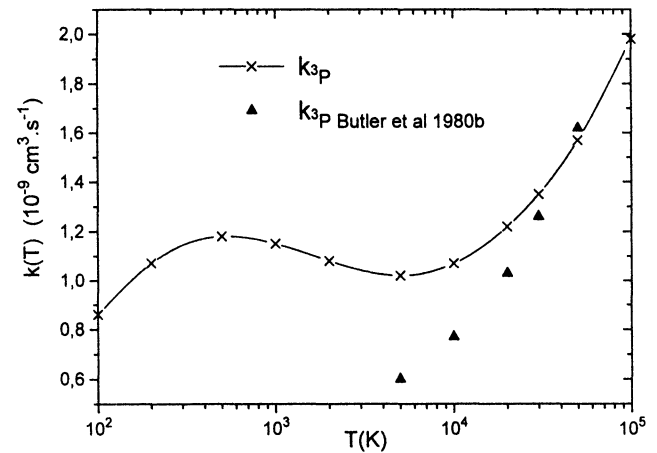


Fig. 3. The rate coefficient k^3P ($10^{-9} \text{ cm}^3 \text{ s}^{-1}$) for charge transfer by 3P ground state O^{2+} ions from atomic H as a function of temperature (K). The crosses refer to the present calculations, the solid triangles to the results of Butler et al. 1980b

easily explained by the minimum energy separations and radial couplings (Sect. 2).

The corresponding rate coefficients k^3P are presented in Table 3 for the temperature range (10^2 – 10^5 K). The variation of k^3P rate with temperature is shown on Fig. 3.

If we compare our results with those of Butler et al. (1980b) (calculated on the basis of Heil et al. cross sections, we find the results are comparable at temperatures of around 50 000 K. But the disagreement between our k^3P and those of Butler et al. widens as the temperature decreases. At 10 000 K, our k^3P is about 50% larger than the value obtained by Butler et al.

In their astrophysical model calculations, Péquignot et al. (1978) treat the k^3P rate coefficient as an empirical parameter optimized to the observed data. In the case of the planetary nebula NGC 7027, they found that the observed spectral data are best reproduced by a temperature of 10 000 K and an empirical

reaction rate coefficient of $1.6 \cdot 10^{-9} \text{ cm}^3 \text{ s}^{-1}$. This value is closer to our calculated rate constant of $1.07 \cdot 10^{-9} \text{ cm}^3 \text{ s}^{-1}$ than to the value $0.77 \cdot 10^{-9} \text{ cm}^3 \text{ s}^{-1}$ obtained by Butler et al..

In 1989 Gruenwald and Péquignot (1989) went a stage further. They obtained evidence for discrepancies between the ionization balance ratio predicted by their photoionization model of NGC 7027 and the observations. They found that their model produced an $[O^+]/[O^{2+}]$ ratio 40% too small by comparison with the observations and concluded that the rate coefficient k^3P of Butler et al. used in their model I must be too small. The temperature used in their model was approximately 14 000 K. At this temperature our reaction rate coefficient is 25% larger than that of Butler et al. (Table 3).

However, Middlemass (1990) recently advanced that k^3P need not be as large as Péquignot et al. and Gruenwald and Péquignot propose. Indeed in his planetary nebula NGC 7027 model, Middlemass got an average ratio value only 20% smaller than the observed one – but with a spread based on individual lines which suggests the predicted/observed ratio is between 1.2 and 0.6.

In some more recent calculations on NGC 7027, Péquignot (private communication 1994) has reassessed the rate coefficient compatible with his model and the latest observations. He finds a rate coefficient of $(1.4 \pm 0.3) \cdot 10^{-9} \text{ cm}^3 \text{ s}^{-1}$ at a temperature of 13 000 K. Our calculated value is just within the lower error bar limit.

4. Conclusion

At thermal energies, it is confirmed that the charge transfer reaction of $O^{2+}(^3P)$ ions with atomic H is fast, producing O^+ ions in the excited $(2s,2p^4)^4P$ state while metastable 1D state O^{2+} ions react only weakly with atomic H. Our calculated rate coefficients are in satisfactory agreement with recent photoionization models, even though these models cannot be expected to provide an absolute standard. It would be interesting to test our calculated rate constants on the $[O^+]/[O^{2+}]$ ratio in low temperature objects such as the nova shell DQ Herculis 1934 (Petitjean et al. 1990).

Acknowledgements. The authors wish to express their thanks to Dr. Daniel Péquignot for making available his results in advance of publication.

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