

CHARGE EXCHANGE AND FINE STRUCTURE EXCITATION IN O-H⁺ COLLISIONS

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INTRODUCTION

The charge-transfer reaction between protons and oxygen atoms is critical to the chemistry of the oxygen family; the corresponding rate was evaluated by Field and Steigman (1971) on the assumption of orbiting collisions and statistical probability distribution among the levels. We re-examine this reaction, including the fine-structure excitation process, basing our analysis on a careful description of the different potential curves arising from the O-H⁺ and O⁺-H systems and on the evaluation of the coupling responsible for the transitions.

INTERATOMIC POTENTIALS

The charge-transfer reaction is almost resonant; the energy defects between the different exit channels are displayed in Table 1 (below):

Table 1

States	Energy (K)
O (³ P ₂) + H ⁺	0
O ⁺ (⁴ S _{3/2}) + H	227
O (³ P ₁) + H ⁺	228
O (³ P ₀) + H ⁺	326

Such an accuracy in the relative position of potential energy curves is not available from even the most elaborate ab-initio calculations. In order to avoid this difficulty, we chose to use the experimental values of the energies of the separated atoms limit, use the classical asymptotic behaviours, and join them to the results given by Liu and Verhaegen (1971) at short internuclear distances, since these authors were able to obtain the correct asymptotic energies by an estimation of the correlation energies. For the O-H⁺ system, when neglecting fine-structure effects, we have two potential curves X ³Σ⁻ and A ³Π. The asymptotic behaviour is due to a first order charge-quadrupole term varying as

$1/R^3$ and a second order charge-dipole interaction varying as $1/R^4$. For the O^+-H system, two molecular potentials are involved, $^5\Sigma^-$ and $^3\Sigma^-$. For the $^5\Sigma^-$ curve, the long range interaction is due to the attractive charge-dipole interaction in $1/R^4$ and an additive repulsive term evaluated with valence bond functions and expressed in an exponential form. The $^3\Sigma^-$ potential was determined through the energy difference between the $^5\Sigma^-$ and $^3\Sigma^-$ potentials, which is given in terms of exchange integrals numerically determined for large internuclear distances ($R > 6$ a.u.).

THE COLLISION TREATMENT

At the low energies of the interstellar medium, a full quantum mechanical solution of the scattering problem is required to achieve a satisfactory treatment.

We performed close-coupling calculations, expanding the total wave function in the symmetric-top wave functions, using the formalism described by Mies (1973) for fine-structure transitions. When the charge-exchange channel is taken into account, the couplings between different electronic configurations must also be considered. We neglected the rotational coupling and the fine-structure coupling between different electronic configurations. We kept the fine-structure coupling inside the $O(^3P)-H^+$ configuration, and by numerical calculations involving bielectronic integrals we determined the electronic coupling between the two $^3\Sigma^-$ states that is essentially responsible for the charge-exchange reaction.

RESULTS

We determined the cross sections for different energies and performed a Maxwell average over the velocities in order to obtain the corresponding rate-constants. The results are given in Table 2 for various temperatures; they are noticeably different from the previous estimates of Field and Steigman (1971). Indeed the orbiting approximation is questionable for this system because of the large energy defect which must be surmounted in inelastic collisions and because of the quadrupolar coupling between fine-structure levels at large distances.

Table 2 - Rate constants in $10^{-9} \text{ cm}^3\text{s}^{-1}$ (k)

	<u>T(K)30</u>	<u>T(K)50</u>	<u>T(K)70</u>	<u>T(K)100</u>	<u>T(K)1000</u>
$k_2 \rightarrow 3/2$	$6.30 \cdot 10^{-5}$	$1.38 \cdot 10^{-3}$	$5.31 \cdot 10^{-3}$	$1.52 \cdot 10^{-2}$	$4.77 \cdot 10^{-1}$
$k_2 \rightarrow 1$	$9.10 \cdot 10^{-5}$	$2.02 \cdot 10^{-3}$	$8.07 \cdot 10^{-3}$	$2.42 \cdot 10^{-2}$	$9.42 \cdot 10^{-1}$
$k_2 \rightarrow 0$	$1.44 \cdot 10^{-7}$	$1.69 \cdot 10^{-5}$	$1.51 \cdot 10^{-4}$	$8.82 \cdot 10^{-4}$	$1.54 \cdot 10^{-1}$

REFERENCES

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