EFFECTIVE OPERATORS IN CHARGE EXCHANGE STUDIES

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ABSTRACT. The rate coefficient for the charge transfer reaction $C^{+2}P^O + H \rightarrow C\ ^3P + H^+$ is calculated with the introduction of the radial coupling between the two $^3\pi$ states arising from both asymptotic atomic states. The derived rate coefficient at a temperature of 10^4K is $2\ 10^{-15}$ cm³s⁻¹ which is two orders of magnitude larger than the value previously estimated by Butler and Dalgarno (1980) from a weak spin orbit coupling between the $^3\Sigma^-$ and $^3\Sigma^+$ molecular states of CH⁺.

1.   THE EFFECTIVE HAMILTONIAN TECHNIQUE

We describe non B.O. processes in a (non orthogonal) asymptotic basis of the system. We thus define both an effective hamiltonian and an effective operator for the dynamical couplings. (Levy 1982). These operators reproduce the results of an extensive C.I. calculation and are built by mean of a projection technique. Two cases are studied where the number of C.I. eigenvalues are equal or lower to the dimension of the asymptotical basis.
    This technique enables us to calculate the first two $^3\pi$ molecular potentials as well as their electronic coupling in a diabatic basis.

2.   CHARGE TRANSFER CALCULATIONS

We then solve the scattering equations

$$(\frac{h^2}{2\mu} \nabla^2_R \underset{\sim}{I} - \underset{\sim}{V}(R) + E\underset{\sim}{I}) \ F(R) = 0 \tag{1}$$

where $\underset{\sim}{V}(R)$ is the interaction matrix.

The cross section $\sigma(E)$ at an energy E is reduced to a weighted value of $\sigma(^3\pi)$ where $\sigma(^3\pi)$ is the cross section for charge transfer in the $^3\pi$ symmetry calculated from equation (1)

$$\sigma_{C^+ + H \to C + H^+} = \frac{1}{2}\, \sigma_{\to}(^3\pi)$$

$$\sigma_{C^+ + H \leftarrow C + H^+} = \frac{2}{3}\, \sigma_{\leftarrow}(^3\pi)$$

The reaction rate coefficient is then obtained after a maxwellian average over temperature. Table 1 gives the values of the direct and reverse charge transfer reaction rate coefficients for different temperatures ranging from 6000 K to 50 000 K.

At 10 000 K the value is two orders of magnitude larger than that estimated by Butler and Dalgarno (1980) who assume that the reaction takes place via a weak spin-orbit coupling between the $^3\Sigma^+$ and $^3\Sigma^-$ molecular states of CH^+.

TABLE 1.

$k_{C^+ + H \to C + H^+}\ cm^3 s^{-1}$	$k_{C^+ + H \leftarrow C + H^+}\ cm^3 s^{-1}$	T (in K)
$2.5\ 10^{-16}$	$9.05\ 10^{-14}$	6 000
$5.15\ 10^{-16}$	$9.84\ 10^{-14}$	7 000
$9.04\ 10^{-16}$	$1.07\ 10^{-13}$	8 000
$1.42\ 10^{-15}$	$1.15\ 10^{-13}$	9 000
$2.06\ 10^{-15}$	$1.23\ 10^{-13}$	10 000
$2.85\ 10^{-15}$	$1.33\ 10^{-13}$	11 000
$3.80\ 10^{-15}$	$1.45\ 10^{-13}$	12 000
$8.23\ 10^{-15}$	$2.\ \ 10^{-13}$	15 000
$2.87\ 10^{-14}$	$4.44\ 10^{-13}$	20 000
$2.24\ 10^{-14}$	$2.2\ 10^{-12}$	30 000
$8.17\ 10^{-13}$	$6.4\ 10^{-12}$	40 000
$1.98\ 10^{-12}$	$1.36\ 10^{-11}$	50 000

References

S.E. Butler and A. Dalgarno, Astron.Astrophys. 85, 144 (1980).

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