APPLICATIONS OF THE PROBABILITY CURRENT METHOD TO NUCLEAR DYNAMICAL CALCULATIONS IN COLLISIONS WITH HYDROGEN

Ya. V. Voronov [a*], ***A. K. Belyaev*** [a**]

[a] *Department of Theoretical Physics and Astronomy, Herzen University, St. Petersburg, 191186, Russia*

The probability current method is applied for nuclear dynamics treatment of inelastic processes in collisions of heavy atoms and ions with hydrogen atoms and ions, in particular: Li + H, Li^+ + H^-, Ca + H, Ca^+ + H^-, Ca^+ + H, Ca + H^+, Ca^2+ + H^-, O + H, O^- + H^+ and O^+ + H^-. Comparison of the data obtained by different methods (both full quantum and model quantum calculations) shows good agreement for the processes with the large values of the rate coefficients, which are of particular astrophysical interest.

Keywords: atomic data – atomic processes – stars: abundances

1. INTRODUCTION

Non-Local Thermodynamic Equilibrium modeling of stellar spectra requires data on inelastic collisions, especially with hydrogen atoms and ions. Since full calculations (both for ab initio electronic structures and complete nuclear dynamics) are still time-consuming and still complicated in applications to different collisional systems, the classical Drawin's formula for estimating rate coefficients of inelastic processes in hydrogen-collisions provides unreliable data, approximate but reliable model methods are desired.

The probability current method [1, 3] is one of such models. It is developed within the Born-Oppenheimer formalism and based on the Landau-Zener model for determination of a transition probability for a single passage of a non-adiabatic region. An application of this method is especially reasonable when potential energies are calculated by the quantum chemical methods, but non-adiabatic couplings are not computed.

* E-mail: voronov_yaroslav@mail.ru
** E-mail: akbelyaev@herzen.spb.ru

The rates obtained by the probability current method agree with rates calculated by other nuclear dynamical approaches. The method has been applied for studies of inelastic collisions in LiH [2], CaH [3], CaH^+ [4] and OH [5,6] quasimolecules. It is shown that for all considered collisions the largest values of rate coefficients (larger than 10^{-8} cm^3/s) correspond to neutralization processes into final states with the binding energies around -2 eV.

2. RESULTS

2.1. Li + H and Li^+ + H^- collisions

Nuclear dynamic calculations are performed for 7 covalent states and one ionic. The potentials are taken from [7]. The cross sections are calculated for the collisional energy range 0.01–100 eV, the rate coefficients are calculated for the temperature range 1'000–10'000 K with the step 1'000 K.

Comparison of the rate coefficients obtained by the probability current method and by the full quantum calculations [7] for mutual neutralization processes at temperature T = 6'000 K shows good agreement: for the processes into the final channels Li(3s,3p,3d,4p) + H(1s) a difference between these two datasets is less than 19%. The largest rate coefficients (larger than 10^{-8} cm^3/s) corresponds to mutual neutralization processes into the final molecular states Li(3s,3p) + H(1s).

2.2. Ca + H and Ca^+ + H^- collisions

Nuclear dynamics calculations for 10 covalent and one ionic ab initio potentials are performed by the probability current method. The cross sections and the rate coefficients are calculated for the collisional energy range 0.01–100 eV and for the temperature range 1'000–10'000 K with the step 1'000 K, respectively. The largest values of the rate coefficients correspond to the mutual neutralization processes into the final states Ca(4s5s ^{1,3}S, 4s5p ^{1,3}P) and belong to the range $(2.40–5.50)\times10^{-8}$ cm^3/s. Comparison of these data with the rate coefficients, obtained by the full quantum calculations (Belyaev et.al., in press), at the temperature T = 6'000 K for the mutual neutralization processes shows good agreement: difference for the processes $Ca^+ + H^- \rightarrow$ Ca(3d4s ^{1}D), Ca(4s5s ^{1,3}S), Ca(4s5p ^{1,3}P) + H(1s) is less than 33%.

2.3. Ca^+ + H, Ca + H^+ and Ca^2+ + H^- collisions

Nuclear dynamics in CaH^+ collisions is performed for 17 states obtained by quantum chemical calculations in [8]. The cross sections are calculated for the

collisional energy range 0.01–100 eV , and the rate coefficients are calculated for the temperature range 1'000–10'000 K with the step 1'000 K.

The largest values of the rate coefficients correspond to the mutual neutralization processes into the final states $Ca^+(4f, 6s, 5d, 6p, 7s) + H(1s)$, and also to the de-excitation process $Ca(4s4p\ ^1P) + H^+ \rightarrow Ca^+(4s\ ^2S) + H(1s\ ^2S)$ and belong to the range 1.79×10^{-8} – 1.56×10^{-7} cm^3/s.

2.4. O + H, O^- + H^+ and O^+ + H^- collisions

Nuclear dynamic calculations for OH quasimolecule are performed for 11 covalent states and two ionic: $O^-(2p^5\ ^2P) + H^+$ and $O^+(2p^3\ ^4S^\circ) + H^-$, the potentials are taken from [5]. Six molecular symmetries have been treated separately, the total rate coefficients for each inelastic process are calculated as a sum over all molecular symmetries. The cross sections are calculated for the collisional energy range 0.01–100 eV, the rate coefficients are calculated for the temperature range 1'000–10'000 K.The largest values of the rate coefficients (greater than 10^{-8} cm^3/s) at the temperature T = 6'000 K correspond to the mutual neutralization processes $O^-(2p^5\ ^2P) + H^+ \rightarrow O(2p^4\ ^3P) + H(2p\ ^2P)$ (2.56×10^{-8} cm^3/s), $O^+(2p^3\ ^4S^\circ) + H^-(1s^2\ 1S) \rightarrow O(2p^3 3p\ ^3P) + H(1s\ ^2S)$ (1.98×10^{-8} cm^3/s) and $O^+(2p^3\ ^4S^\circ) + H^-(1s^2\ 1S) \rightarrow O(2p^3 4s\ ^5S^\circ) + H(1s\ ^2S)$ (2.95×10^{-8} cm^3/s).

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