Model Approach for Inelastic Processes in Collisions of Heavy Particles with Hydrogen

S.A. Yakovleva[1], A.K. Belyaev[1]

E-mail: *cvetaja@gmail.com*

The quantum model approach within the framework of the Born–Oppenheimer formalism has been recently proposed to evaluate physically reliable data on rate coefficients for inelastic processes in collisions of atoms and positive ions of different chemical elements with hydrogen atoms and negative ions.

1 Introduction

Formation of spectral lines in stellar atmospheres is determined by many physical processes. Collisions of atoms and positive ions of different species with hydrogen atoms and anions are one of the main sources of uncertainties for non-LTE studies due to the high concentration of hydrogen [1].

The best way to get information on the rate coefficients for hydrogen collisions is to carry out full quantum studies. But these calculations are very time-consuming, and only a few collisional partners have already been studied at low collision energies. These are hydrogen collisions with hydrogen [2], helium [3], lithium [4, 5], sodium [6], and magnesium [7].

The data for hydrogen collisions are still rare, so the Drawin formula was widely used to estimate inelastic collision rate coefficients, although it has been shown [8] that the Drawin formula does not provide reliable data and can not be applied to charge transfer processes, which have been found to be the most important in astrophysical applications. A comparison of the rate coefficients obtained in full quantum studies and with the Drawin formula was performed in [8]. The rate coefficients obtained in quantum calculations are not larger than 10^{-8} cm^3/s, while the highest values for estimations by means of the Drawin formula are up to 10^{-2} cm^3/s, which is a huge value for an inelastic rate coefficient. Moreover, this formula gives zero rates for charge transfer processes, such as mutual neutralization and ion pair formation, which have been shown to have one of the largest values according to quantum calculations.

That is why it is important to develop and apply quantum model approaches that would provide reliable data, even approximate. Such quantum model approach for collisions of atoms and positive ions of different chemical elements with hydrogen atoms and negative ions was recently proposed in [9, 10].

[1] Dep. of Theoretical Physics and Astronomy, Herzen University, St. Petersburg, Russia

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2 Quantum model approach

Low-energy atomic collisions are well described within the quantum Born-Oppenheimer approach. Within this framework the problem is solved in two steps. The first step includes electronic structure calculations. It can be based on accurate quantum-chemical data, if available. For many cases, accurate quantum-chemical data are not available, and approximate adiabatic potentials can be constructed via modeling of ionic-covalent interaction as described in [9]. Also it is possible to combine modeled potentials for higher-lying states with available *ab initio* potentials for low-lying states.

The second step includes non-adiabatic nuclear dynamics calculations. In the case, when adjacent states form several non-adiabatic regions, the probability current method described in [9] can be applied. The other option is to use multichannel formulas [10, 11], but they are only applicable for the case of ionic-covalent interaction (every pair of adjacent states form only one non-adiabatic region).

3 Results

The comparison of the results given by the quantum model approach and by full quantum study was performed in [7] for the case of magnesium-hydrogen collisions. Rate coefficients obtained in these studies are shown in Fig. 1.

The vertical axis represents results of the quantum model calculations, while the horizontal axis does results of the full quantum study. The symbols in Fig. 1 correspond to the rate coefficients of the partial processes, associated with

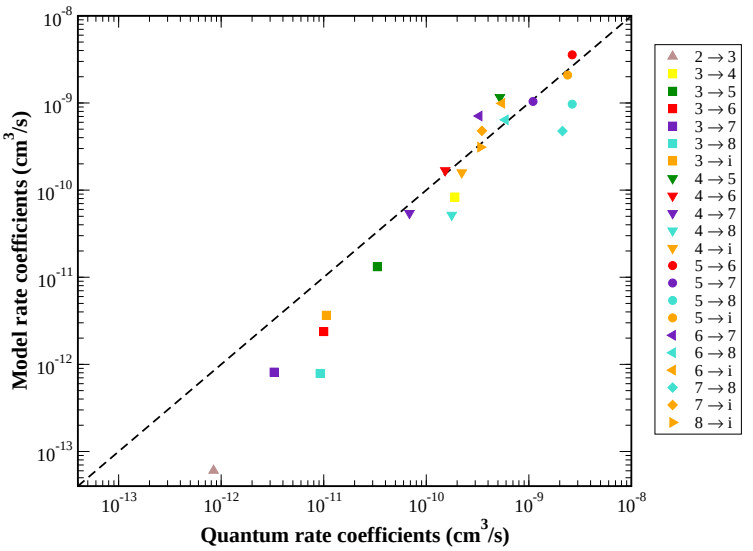

Figure 1: Comparison of the rate coefficients at $T = 6000$ K for the case of Mg-H collisions.

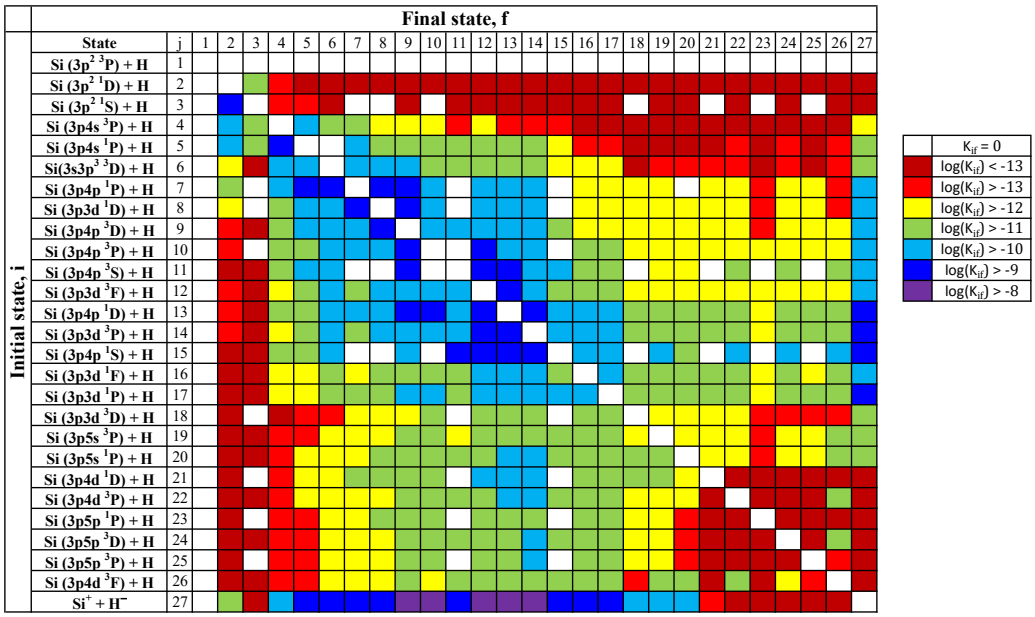

Figure 2: Rate coefficients (in cm^3/s) at $T = 6000\,\mathrm{K}$ for the case of Si-H collisions.

transitions between different molecular states numbered starting from the ground one (the index i corresponds to the ionic state). It is seen that the agreement for the rate coefficients with high and moderate values is quite good. While there are some deviations for the processes with small values of the rate coefficients, for which both the quantum model approach and the full quantum study give negligibly small values.

In [10], the quantum model approach was applied to silicon-hydrogen collisions. These calculations included 27 molecular states, and the heat map with the rate coefficients for different inelastic processes is represented in Fig. 2. The purple squares correspond to the highest rates, while white ones correspond to zero rates. It is seen that the highest values correspond to the charge transfer processes such as mutual neutralization and ion pair formation.

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* The color figures are available online in the Proceedings at *http://www.astro.spbu.ru/sobolev100/*.