

# Estimating inelastic heavy-particle – hydrogen collision data

## II. Simplified model for ionic collisions and application to barium-hydrogen ionic collisions<sup>\*</sup>

Andrey K. Belyaev<sup>1,2</sup> and Svetlana A. Yakovleva<sup>2</sup>

<sup>1</sup> Max-Planck Institute for Astrophysics, Postfach 1371, 85741 Garching, Germany  
e-mail: [andrey.k.belyaev@gmail.com](mailto:andrey.k.belyaev@gmail.com)

<sup>2</sup> Department of Theoretical Physics and Astronomy, Herzen University, 191186 St. Petersburg, Russia

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### ABSTRACT

**Aims.** A simplified model is derived for estimating rate coefficients for inelastic processes in low-energy collisions of heavy particles with hydrogen, in particular, the rate coefficients with high and moderate values. Such processes are important for non-local thermodynamic equilibrium modeling of cool stellar atmospheres.

**Methods.** The derived method is based on the asymptotic approach for electronic structure calculations and the Landau-Zener model for nonadiabatic transition probability determination.

**Results.** It is found that the rate coefficients are expressed via statistical probabilities and reduced rate coefficients. It is shown that the reduced rate coefficients for neutralization and ion-pair formation processes depend on single electronic bound energies of an atomic particle, while the reduced rate coefficients for excitation and de-excitation processes depend on two electronic bound energies. The reduced rate coefficients are calculated and tabulated as functions of electronic bound energies. The derived model is applied to barium-hydrogen ionic collisions. For the first time, rate coefficients are evaluated for inelastic processes in  $\text{Ba}^+ + \text{H}$  and  $\text{Ba}^{2+} + \text{H}^-$  collisions for all transitions between the states from the ground and up to and including the ionic state.

**Key words.** atomic data – atomic processes – stars: atmospheres

### 1. Introduction

Non-local thermodynamic equilibrium (non-LTE) modelings of different astrophysical phenomena are important for many fundamental problems in modern astrophysics (see, e.g., reviews [Asplund 2005](#); [Mashonkina 2014](#); [Barklem 2016a](#), and references therein). In particular, non-LTE modelings of stellar atmospheres are of importance, for example, for determining absolute and relative abundances of various chemical elements, for the Galactic evolution, and so on. Non-LTE modeling requires detailed and complete information about inelastic heavy-particle collision processes, most importantly those in collisions with hydrogen atoms and negative ions. The lack of atomic data on inelastic processes due to collisions with neutral hydrogen atoms and hydrogen negative ions has been a major limitation on non-LTE modeling of stellar spectra. This problem has been well documented (see, e.g., [Lambert 1993](#); [Asplund 2005](#); [Mashonkina 2014](#); [Barklem 2016a](#), and references therein). Recently, significant progress has been achieved through detailed full quantum scattering calculations based on accurate ab initio quantum chemical data for the cases of simple atoms, such as He, Li, Na, Mg, and Ca ([Belyaev et al. 1999, 2010, 2012](#); [Croft et al. 1999a,b](#); [Belyaev & Barklem 2003](#); [Guitou et al. 2011, 2015](#); [Belyaev 2015](#); [Mitrushchenkov et al. 2017](#)). This allowed one to perform accurate non-LTE modeling of stellar spectra ([Barklem et al. 2003](#); [Lind et al. 2011](#); [Osorio & Barklem 2016](#); [Mashonkina et al. 2017](#)). Nevertheless, full quantum ab initio and scattering calculations are still time consuming and, hence, rather seldom.

Owing to high demand in atomic data for inelastic processes in collisions with hydrogen and a large number of partial processes and atomic states to be taken into account, astrophysicists were forced to use widely the classical Drawin formula ([Drawin 1968, 1969](#); [Drawin & Emard 1973](#); [Steenbock & Holweger 1984](#); [Lambert 1993](#)). Later on, it was recognized that the Drawin formula is not reliable ([Barklem et al. 2011](#); see also [Asplund 2005](#)), and it was emphasized that it is highly desirable to derive an approximate model approach to inelastic atomic collisions with hydrogen. Low computational cost are also considered important.

In non-LTE modelings many other processes, including radiative processes and other collisional processes, especially those with electrons, are taken into account. A collisional process with hydrogen is only of importance, if the rate coefficient is comparable to those for the other processes (see, e.g., [Mashonkina 2014](#); [Barklem 2016a](#)). Thus, a desirable model approach to inelastic collisions with hydrogen should provide rate coefficients with high and moderate values.

Two such approaches for nonadiabatic nuclear dynamics have been proposed: the quantum branching probability current method ([Belyaev 2013a](#)) and the quantum multichannel analytic approach ([Belyaev 1993](#); [Belyaev & Barklem 2003](#); [Belyaev et al. 2014](#); [Yakovleva et al. 2016](#)). Both approaches are based on electronic structure calculations and the Landau-Zener model. For electronic structure calculations, in addition to ab initio methods, the approximate methods have been used: the asymptotic method ([Belyaev 2013a](#)) and the Linear Combinations of Atomic Orbitals (LCAO) method ([Barklem 2016b, 2017](#)). The quantum model approaches have been successfully applied to a number of chemical elements relevant to non-LTE modeling, such as Al, Si, Ca, Be, and Mn,

<sup>\*</sup> Tables with calculated data are only available at the CDS via anonymous ftp to [cdsarc.u-strasbg.fr](http://cdsarc.u-strasbg.fr) (130.79.128.5) or via <http://cdsarc.u-strasbg.fr/viz-bin/qcat?J/A+A/608/A33>

(Belyaev 2013b; Belyaev et al. 2014, 2016; Yakovleva et al. 2016; Barklem 2016b, 2017; Belyaev & Voronov 2017).

Although the approximate model calculations are less time-consuming than the full quantum calculations, they still require some computation. For this reason, the simplified model for inelastic atomic collisions with hydrogen has been proposed very recently (Belyaev & Yakovleva 2017); hereafter, we refer to this paper to as Paper I. The simplified model practically does not require any computational efforts. In the present paper, the simplified model is extended on inclusion of inelastic ionic collisions with hydrogen and applied to barium-hydrogen ionic collisions, which are of astrophysical interest (Asplund 2005).

## 2. Simplified model for estimating inelastic collision rate coefficients

### 2.1. General description

Let us consider a general case of collisions of  $A^{Z+} + H$  and  $A^{(Z+1)+} + H^-$ , where  $A$  is a chemical element of interest and  $Z = 0, 1, \dots$  is a charge of this element. The case  $Z = 0$  corresponds to atomic collisions with hydrogen,  $Z \geq 1$  to ionic collisions. The heavy-particle  $A^{Z+}$  can be in the ground and in excited states. The main goal of the present model is to estimate high-valued inelastic rate coefficients in collisions with hydrogen, which occur in non-LTE stellar atmosphere modeling.

We are interested in inelastic collision processes that change electronic states of atomic (ionic) particles, nevertheless, theoretical treatments of low-energy atomic and ionic collisions are performed within the molecular representation, and reaction mechanisms are based on nonadiabatic transitions between molecular states. It has been proven by full quantum calculations (see Belyaev et al. 1999, 2010, 2012; Croft et al. 1999a,b; Belyaev & Barklem 2003) that the rate coefficients with high and moderate values are determined by long-range nonadiabatic transitions due to the interactions between  $A^{(Z+1)+} + H^-$  ionic and  $A^{Z+}(j) + H$  covalent molecular states. The index  $j$  denotes an electronic state of  $A^{Z+}$ . So, one needs to determine molecular state symmetries that lead to rates with high values. These symmetries are those which correspond to ionic molecular states. Within the  $LS$  coupling scheme, molecular states are determined by symmetries such as a total spin quantum number  $S$  and an absolute value of a projection quantum number of total orbital electronic angular momentum  $\Lambda$  and other quantum numbers. Since the  $H^-$  anion has the  $^1S$  symmetry, the spin quantum number  $S$  of the ionic molecular state has a single value, while  $\Lambda$  can have several values, and both quantum numbers are uniquely determined by the ground state of the  $A^{(Z+1)+}$  ion.

As pointed out in Paper I, the rate coefficients  $K_{if}$  for an inelastic process  $i \rightarrow f$  can be expressed via the reduced rate coefficients  $N_{if}^\Lambda$  for neutralization and ion-pair formation processes

$$K_{if}(T) = \sum_{\Lambda} p_i^{\text{stat},\Lambda} N_{if}^\Lambda(T; E_f), \quad (1)$$

or via  $D_{if}^\Lambda$  for (de-)excitation processes

$$K_{if}(T) = \sum_{\Lambda} p_i^{\text{stat},\Lambda} D_{if}^\Lambda(T; E_i, E_f), \quad (2)$$

where  $p_i^{\text{stat},\Lambda}$  a statistical probability for population of the initial molecular state  $i$  with a given molecular symmetry  $\Lambda$  from a scattering channel and  $T$  is a temperature. The sums in these

equations are taken over all possible quantum numbers  $\Lambda$  corresponding to the ground ionic molecular state  $A^{(Z+1)+} + H^-$ . The energy  $E_j$  is an electronic bound energy<sup>1</sup> of an  $A^{Z+}(j)$  state to which a molecular state asymptotically corresponds. Although the spin  $S$  and other quantum numbers do not appear explicitly, these values are needed to select covalent molecular states that are populated during a collision and, hence, for selecting final atomic (ionic)  $A^{Z+}(f)$  states populated.

For estimating rate coefficients  $K_{if}(T)$ , the reduced rate coefficients  $N_{if}^\Lambda(T; E_f)$  and  $D_{if}^\Lambda(T; E_i, E_f)$  must be known for each molecular symmetry of interest. The statistical probabilities  $p_j^{\text{stat},\Lambda}$  can be readily calculated. It turns out that within some reasonable approximations (see below) the reduced rate coefficient  $N_{if}^\Lambda(T; E_f)$  for the neutralization process  $A^{(Z+1)+} + H^- \rightarrow A^{Z+}(f) + H$  depends on a single bound energy  $E_f \equiv E_{A^{Z+}(f)}$ , while the reduced rate coefficient  $D_{if}^\Lambda(T; E_i, E_f)$  for the (de-) excitation process  $A^{Z+}(i) + H \rightarrow A^{Z+}(f) + H$  depends on two electronic bound energies,  $E_i \equiv E_{A^{Z+}(i)}$  and  $E_f \equiv E_{A^{Z+}(f)}$ .

Thus, in order to estimate a rate coefficient for a particular process with participation a particular chemical element, one must know the dependence of a corresponding reduced rate coefficient on bound energies. Such dependences are provided by the present simplified model. The reduced rate coefficients for the case  $Z = 0$  are calculated and tabulated as functions of electronic bound energies in Paper I. The cases  $Z = 1, 2$  are treated in the present paper together with the general derivations and an application to barium-hydrogen ionic collisions.

The rate coefficients for exothermic processes (neutralization and de-excitation) depend weakly on the temperature, while the rates for inverse endothermic processes (ion-pair formation and excitation) depend strongly on the temperature. Taking this into account, it is better first to calculate the rate coefficients  $K_{jk}(T)$  for exothermic processes ( $j \rightarrow k$  transitions) and then to calculate the rate coefficients  $K_{kj}(T)$  for the inverse endothermic processes ( $k \rightarrow j$  transitions) by means of the detailed balance relation

$$K_{kj}(T) = K_{jk}(T) \frac{p_k^{\text{stat}}}{p_j^{\text{stat}}} \exp\left(-\frac{\Delta E_{jk}}{k_B T}\right), \quad (3)$$

where  $\Delta E_{jk} = E_j - E_k$  is the energy defect of the process. One should note that for exothermic ( $j \rightarrow k$ ) processes  $\Delta E_{jk}$  is positive.

### 2.2. Reduced rate coefficients for neutralization and ion-pair formation processes

Within a molecular symmetry  $\Lambda$ , a reduced rate coefficient  $N_{if}^\Lambda(T; E_f)$  for the neutralization process  $A^{(Z+1)+} + H^- \rightarrow A^{Z+}(f) + H$  is calculated by integrating a partial cross section  $\sigma_{if}^{N,\Lambda}(E)$  for the process with the Maxwell distribution

$$N_{if}^\Lambda(T; E_f) = \sqrt{\frac{8}{\pi\mu(k_B T)^3}} \int_0^\infty \sigma_{if}^{N,\Lambda}(E) E \exp\left(-\frac{E}{k_B T}\right) dE, \quad (4)$$

where  $E$  is the collision energy,  $k_B$  the Boltzmann constant, and  $\mu$  the reduced nuclear mass. In turn, the neutralization cross section

<sup>1</sup> An electronic bound energy  $E_j$  is measured from an ionization limit of  $A^{Z+}$ , and, hence, it is negative. If an electronic energy  $\tilde{E}_j$  is measured from a ground-state energy of  $A^{Z+}$  as a zero-energy level, then the electronic bound energy should be recalculated as  $E_j = \tilde{E}_j - I_{\text{ionization}}$ , where  $I_{\text{ionization}}$  is an ionization potential of  $A^{Z+}$ .

is calculated as a sum over total angular momentum quantum number  $J$

$$\sigma_{if}^{N,\Lambda}(E) = \frac{\pi\hbar^2}{2\mu E} \sum_{J=0}^{J_{\max}} P_{if}^{N,\Lambda}(J, E) (2J+1), \quad (5)$$

where  $P_{if}^{N,\Lambda}$  is a probability for a state-to-state transition from the initial state  $i = \text{ionic}$  to the final state  $f$  at a given collision energy  $E$  and a given quantum number  $J$ .

In order to estimate state-to-state transition probabilities leading to rates with high values, one needs to know long-range ionic  $A^{(Z+1)+} + H^-$  and covalent  $A^{Z+}(j) + H$  diabatic molecular potentials  $H_{\text{ionic ionic}}$  and  $H_{jj}$  as functions of the internuclear distance  $R$ . These are the Coulomb potential for an ionic molecular state

$$H_{\text{ionic ionic}}(R) = E_{H^-} - \frac{Z+1}{R} \quad (6)$$

and the flat potentials<sup>2</sup> for covalent molecular states

$$H_{jj}(R) = E_j. \quad (7)$$

The electronic bound energy  $E_{H^-}$  for a hydrogen anion is equal to  $-0.754$  eV. These potential energy curves are plotted in Fig. 1. In a general case, the ionic potential crosses several covalent potentials creating a number of nonadiabatic regions; see Fig. 1a. A center  $R_j$  of each nonadiabatic region created by the ionic molecular state and the  $j$ th covalent molecular state is readily determined by equating potentials (6) and (7), and finally is written as

$$R_j = \frac{Z+1}{E_{H^-} - E_j}. \quad (8)$$

Thus, it is seen that a center of a nonadiabatic region is uniquely determined by a corresponding electronic bound energy.

In a multichannel case, a state-to-state transition probability can be calculated by the multichannel formula (Belyaev 1993), which requires information about an energy spectrum of  $A^{Z+}$ . The spectra are different for different chemical elements. However, the state-to-state transition probability  $P_{if}^{N,\Lambda}(J, E)$  for neutralization can be evaluated by a probability calculated in the two-channel approximation depicted in Fig. 1b, that is, one ionic channel and only one covalent  $f$  channel. This approximation does not require information about the whole spectrum but only about the energy level  $f$ . In this case the probability  $P_{if}^{N,\Lambda}(J, E)$  is expressed via a nonadiabatic transition probability  $p_f$ , after a single-pass traversal through the nonadiabatic region  $f$  formed by the ionic state and the final state  $f$ , as follows:

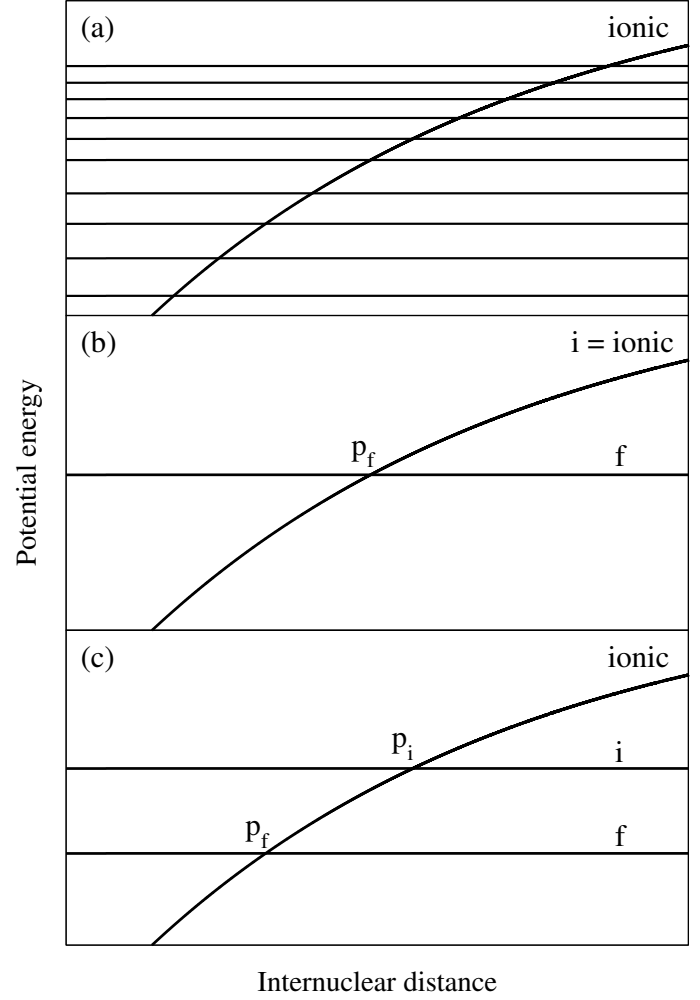
$$P_{if}^{N,\Lambda}(J, E) = 2p_f(1 - p_f). \quad (9)$$

The nonadiabatic transition probability  $p_j$  can be calculated within the Landau-Zener model as follows:

$$p_j \equiv p_{\text{ionic } j} = \exp\left(-\frac{2\pi H_{\text{ionic } j}^2}{\hbar |H'_{\text{ionic ionic}} - H'_{jj}|v}\right), \quad (10)$$

where  $H_{\text{ionic } j}$  is an off-diagonal matrix element for the (diabatic) ionic-covalent interaction,  $v$  is a radial velocity of colliding

<sup>2</sup> In principle, the polarization potentials can be used for ion-atom interactions, but for large  $R$  this gives negligible corrections.



**Fig. 1.** Schematic diagrams of a series of ionic (Coulomb) and covalent potentials in the diabatic representation. *Panel a:* depicts a general multichannel case, *panel b:* a two-channel case (neutralization), and *panel c:* a three-channel case (de-excitation).

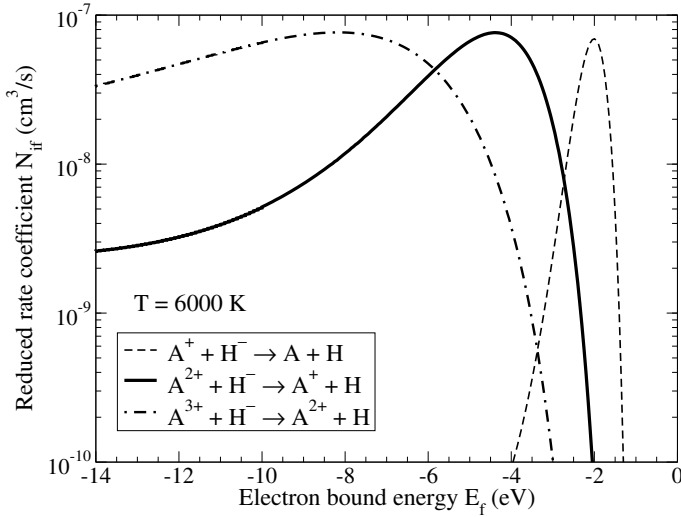
heavy particles, and primed values are referred to as a derivative with respect to the internuclear distance  $R$ . All values are evaluated at the center of the nonadiabatic region  $R_j$ ; see Eq. (8). Substituting the ionic diabatic potential (6) and the covalent diabatic potential (7), and the expression (8) for  $R_j$  into Eq. (10), one can rewrite the formula for the Landau-Zener probability

$$p_j = \exp\left(-\frac{2\pi H_{\text{ionic } j}^2 (Z+1)}{(E_{H^-} - E_j)^2 \hbar v}\right). \quad (11)$$

The off-diagonal matrix element  $H_{\text{ionic } j}$  can be evaluated by the semiempirical formula for one-electron transition charge exchange from Olson et al. (1971), i.e.,

$$H_{\text{ionic } j} = \frac{\sqrt{-E_j} + \sqrt{-E_{H^-}}}{\sqrt{2}} \sqrt{E_j E_{H^-}} R_j \times \exp\left(-0.86 R_j \frac{\sqrt{-E_j} + \sqrt{-E_{H^-}}}{\sqrt{2}}\right). \quad (12)$$

For the neutralization process the initial state is *ionic* and the final state  $f$ , so the index  $j$  in Eqs. (7), (8), (10)–(12) should be



**Fig. 2.** General dependence of neutralization reduced rate coefficients on a final electronic bound energy  $E_f$  obtained by means of the present simplified model at  $T = 6000$  K.

replaced by the index  $f$ . The radial velocity in the nonadiabatic region formed by the ionic state and the final state  $f$  reads

$$v = v_f^N = \sqrt{\frac{2}{\mu} \left( E + E_{H^-} - E_f - \frac{J(J+1)\hbar^2}{2\mu R_f^2} \right)}. \quad (13)$$

It is seen that the state-to-state transition probability  $P_{if}^{N,\Lambda}(J, E)$ , Eq. (9), for a neutralization process at a given collision energy  $E$  and at given quantum number  $J$  is uniquely determined by a single electronic bound energy  $E_f$ . This means that the reduced rate coefficient  $N_{if}^\Lambda(T; E_f)$  for neutralization at a given temperature  $T$  also depends on a single electronic bound energy  $E_f$ .

If the reduced rate coefficient  $N_{jk}^\Lambda(T; E_k)$  for the exothermic neutralization process ( $j \rightarrow k$  transitions; for neutralization processes  $j = \text{ionic}$  is known, then the rate coefficient  $N_{kj}^\Lambda(T; E_k)$  for the inverse endothermic ion-pair formation process ( $k \rightarrow j$  transitions) can be calculated by means of the following detailed balance relation:

$$N_{kj}^\Lambda(T; E_k) = N_{jk}^\Lambda(T; E_k) \exp\left(-\frac{\Delta E_{jk}}{k_B T}\right). \quad (14)$$

This relation is readily derived from Eqs. (1)–(3).

Thus, Eqs. (4)–(14) allow us to calculate the reduced rate coefficients  $N_{if}^\Lambda(T; E_f)$  for neutralization and ion-pair formation processes as a function of an electronic bound energy  $E_f$  at a given temperature  $T$ . Within the simplified model the reduced rates do not depend on  $\Lambda$ , but this quantum number selects which final states are populated from the ionic state within this molecular symmetry. The neutralization reduced rate coefficient for the case  $Z = 0$  is calculated in Paper I and for the cases  $Z = 1, 2$  in the present paper. The results are published at the CDS for the temperature range  $T = 1000$ – $10\,000$  K. For the temperature  $T = 6000$  K the neutralization reduced rate coefficients  $N_{if}(T = 6000; E_f)$  are shown in Fig. 2.

It is seen in this figure that the neutralization reduced rate coefficient for  $Z = 0$  (dashed curve) reaches the maximum value  $6.8 \times 10^{-8} \text{ cm}^3/\text{s}$  at the bound energy  $E_f = -2$  eV. Also, within

the most optimal window<sup>3</sup>  $[-2.7, -1.5]$  eV the reduced rates have high values above  $10^{-8} \text{ cm}^3/\text{s}$ , while within the less optimal window (roughly  $[-4.0, -1.3]$  eV) the reduced rates have moderate values above  $10^{-10} \text{ cm}^3/\text{s}$ , down to nearly three orders of magnitude lower than the maximum value (see Paper I). Outside of these optimal windows the reduced rates have negligible values.

For the case of ionic collisions the behavior of the reduced rate coefficients is different. For  $Z = 1$  the neutralization reduced rate coefficient (solid line) has the broad maximum of  $7.6 \times 10^{-8} \text{ cm}^3/\text{s}$  at the bound energy  $E_f = -4.4$  eV. The most optimal window in these collisions can be estimated by the interval  $[-2.8, -8.3]$  eV for the bound energy, while the less optimal window corresponds to the bound energies  $< -2.1$  eV. For the case of  $Z = 2$ , the neutralization reduced rate (dash-dotted curve) has even broader maximum of  $7.7 \times 10^{-8} \text{ cm}^3/\text{s}$  at the bound energy  $E_f = -8.2$  eV. The most optimal window in these collisions corresponds to the electronic bound energies  $< -4.5$  eV, while the less optimal window  $< -3$  eV. Thus, one may conclude that the optimal windows for neutralization are shifted in the direction toward deeper bound energies with increasing the charge of positive ion in collisions with hydrogen negative ions.

### 2.3. Reduced rate coefficients for de-excitation and excitation processes

Within a molecular symmetry  $\Lambda$ , a reduced rate coefficient  $D_{if}^\Lambda(T; E_i, E_f)$  for the de-excitation process  $A^{Z+}(i) + H \rightarrow A^{Z+}(f) + H$  is calculated by integrating a de-excitation cross section  $\sigma_{if}^{D,\Lambda}(E)$  with the Maxwell distribution

$$D_{if}^\Lambda(T; E_i, E_f) = \sqrt{\frac{8}{\pi\mu(k_B T)^3}} \int_0^\infty \sigma_{if}^{D,\Lambda}(E) E \exp\left(-\frac{E}{k_B T}\right) dE. \quad (15)$$

The de-excitation cross section is calculated as a sum over total angular momentum quantum number  $J$ ,

$$\sigma_{if}^D(E) = \frac{\pi\hbar^2}{2\mu E} \sum_{J=0}^{J_{\max}} P_{if}^{D,\Lambda}(J, E) (2J+1), \quad (16)$$

where  $P_{if}^{D,\Lambda}$  is a probability for a transition from an initial state  $i$  to a final state  $f$ .

Within the same approximation as that used in the previous subsection, the de-excitation reaction mechanism is determined by minimum three diabatic molecular states: two covalent states  $i$  and  $f$ , and one ionic state, as depicted in Fig. 1c. Therefore, there are two nonadiabatic regions that are responsible for the state-to-state transition probability; that is,  $P_{if}^{D,\Lambda}(J, E)$  is expressed via two nonadiabatic transition probabilities,  $p_i$  and  $p_f$ , as follows:

$$P_{if}^{D,\Lambda}(J, E) = 2p_f(1-p_f)(1-p_i). \quad (17)$$

Each probability  $p_i$  and  $p_f$  is after a single-pass traversal through a nonadiabatic region formed by the ionic state and the initial or

<sup>3</sup> By ‘‘an optimal window’’ we mean an electronic energy interval for atomic or ionic states whose participation in inelastic collision processes leads to relatively high rate coefficients. We also define ‘‘the most optimal window’’ as rate coefficient values exceeding  $10^{-8} \text{ cm}^3/\text{s}$  and ‘‘the least optimal window’’ as rate coefficient values exceeding  $10^{-10} \text{ cm}^3/\text{s}$ .



final state  $i$  or  $f$ , and can be calculated within the Landau-Zener model by means of Eqs. (11), (12); see also Eq. (8). In these formulas the index  $j$  should be replaced by indices  $i$  or  $f$  for probabilities  $p_i$  or  $p_f$ , respectively. The radial velocities for de-excitation in the nonadiabatic regions  $i$  and  $f$  read, respectively,

$$v = v_i^D = \sqrt{\frac{2}{\mu} \left( E - \frac{J(J+1)\hbar^2}{2\mu R_i^2} \right)}, \quad (18)$$

$$v = v_f^D = \sqrt{\frac{2}{\mu} \left( E + E_i - E_f - \frac{J(J+1)\hbar^2}{2\mu R_f^2} \right)}. \quad (19)$$

Finally, one can see that the state-to-state transition probability  $P_{if}^{D,\Lambda}$  and the reduced rate coefficient  $D_{if}^\Lambda$  for de-excitation depend on two electronic bound energies  $E_i$  and  $E_f$ .

Thus, Eqs. (8), (11), (12), and (15)–(19) allow us to calculate the reduced rate coefficients  $D_{if}^\Lambda(T; E_i, E_f)$  for de-excitation processes at a given temperature  $T$  as a function of an electronic bound energies  $E_i$  and  $E_f$ . The reduced rates for excitation processes can be calculated from  $D_{if}^\Lambda(T; E_i, E_f)$  by means of the detailed balance relation similar to Eq. (14) replacing  $N$  by  $D$ .

The (de-)excitation reduced rate coefficient for the case  $Z = 0$  is calculated and discussed in Paper I and for the cases  $Z = 1, 2$  in the present paper. The results are published at the CDS for the temperature range  $T = 1000$ – $10\,000$  K. For  $Z = 1$  and for the temperature  $T = 6000$  K the (de-)excitation reduced rate coefficient  $D_{if}(T = 6000; E_i, E_f)$  is shown in Fig. 3.

The (de-)excitation reduced rate coefficient for  $Z = 1$  reaches the maximum value  $1.1 \times 10^{-8}$  cm<sup>3</sup>/s at the bound energies  $E_i \approx E_f \approx -4$  eV. The most optimal window (exceeding the value  $10^{-8}$  cm<sup>3</sup>/s) is located in a narrow vicinity around this point. The less optimal window (exceeding the value  $10^{-10}$  cm<sup>3</sup>/s) is roughly  $[-8, -2.2]$  eV for  $E_i$  and  $< -2.4$  eV for  $E_f$ .

#### 2.4. Summary of the simplified model

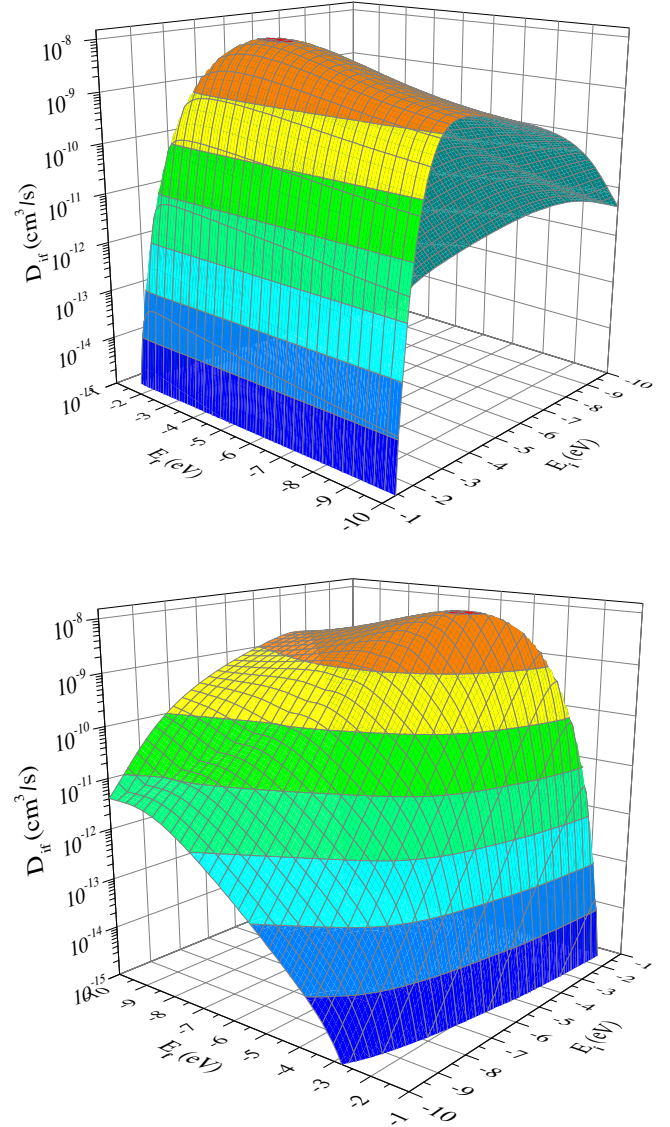
In summary, to estimate the rate coefficients of inelastic processes in collisions with hydrogen by means of the simplified method proposed in the present paper, the following simple steps should be performed:

Step 1. Determining a molecular symmetry for the ground ionic (diabatic)  $A^{(Z+1)+} + H^-$  molecular state within the  $LS$  scheme, i.e., determining a total electronic spin  $S$ , an electronic orbital projection quantum number  $\Lambda$ , and other quantum numbers, if necessary. The values  $S$  and  $\Lambda$  for the ground ionic molecular state are uniquely determined by the ground state of a cation  $A^{(Z+1)+}$ , since an anion  $H^-(^1S)$  has both spin and orbital quantum numbers equal to zero;  $S$  has a single value,  $\Lambda$  might have several values.

Step 2. Determining  $A^{Z+}(j)$  states, which produce covalent  $A^{Z+}(j) + H$  molecular states of the same symmetry as the ground ionic state determined in Step 1, and which correspond to one-electron transitions for the ionic-covalent interaction, i.e., between the  $A^{(Z+1)+} + H^-$  and  $A^{Z+}(j) + H$  (diabatic) states. The electronic bound energies  $E_j$  for the selected atomic/ionic states  $A^{Z+}(j)$  must be determined, for example, from the NIST database.

Step 3. This step is slightly different for the neutralization and de-excitation processes.

Step 3a for neutralization processes  $A^{(Z+1)+} + H^- \rightarrow A^{Z+}(f) + H$ . For a particular final state  $A^{Z+}(f)$ , the corresponding electronic bound energy  $E_f$  is taken and then used



**Fig. 3.** Excitation and de-excitation reduced rate coefficient  $D_{if} \equiv D_{if}^\Lambda(T; E_i, E_f)$  for  $Z = 1$  as a function of the electronic bound energies  $E_i$  and  $E_f$  for the temperature  $T = 6000$  K. The bound energies are measured from the ionization limit. These two subfigures present the same surface for the reduced rate  $D_{if}$  shown from different view points.

to determine the corresponding reduced rate coefficient  $N_{if}$  from the tabulated function  $N_{if}(E_f)$  presented in Fig. 2 for  $T = 6000$  K and provided in the supplementary material for  $T = 1000$ – $10\,000$  K; in other words,  $N_{if} = N_{if}(E_f)$  is determined from the calculated function  $N_{if}(T; E_f)$  for a given temperature  $T$ .

Step 3b for de-excitation processes  $A^{Z+}(i) + H \rightarrow A^{Z+}(f) + H$ . For a particular initial state  $A^{Z+}(i)$  and a particular final state  $A^{Z+}(f)$ , the corresponding electronic bound energies  $E_i$  and  $E_f$  are taken and then used to determine the corresponding reduced rate coefficient  $D_{if}$  from the tabulated function  $D_{if}(E_i, E_f)$  presented in Fig. 3 as the two-dimensional (2D) surface for  $T = 6000$  K and provided in the supplementary material for  $T = 1000$ – $10\,000$  K; in other words,  $D_{if} = D_{if}(E_i, E_f)$  is determined from the calculated function  $D_{if}(T; E_i, E_f)$  for a given temperature  $T$ . This can be performed in one step by using the 2D function  $D_{if}(E_i, E_f)$  or in two steps by first taking a cut of the 2D function  $D_{if}(E_i, E_f)$  at a given bound energy  $E_i$  for the

initial state  $A^{Z+}(i)$  and then by treating the 1D function  $D_{if}(E_f)$  at the given bound energy  $E_f$ ;

Step 4. In order to get the rate coefficient for the neutralization or de-excitation processes, a statistical probability for the population of the initial molecular state is calculated and the reduced rate is multiplied by this statistical probability according to Eqs. (1) or (2), respectively. If the ground ionic  $A^{(Z+)+} + H^-$  molecular state corresponds to various molecular symmetries (several  $\Lambda$ ), then a sum over  $\Lambda$  should be taken. In order to get the rate coefficient for ion-pair formation or for excitation processes, the rate coefficient is calculated for an inverse process from the corresponding rate coefficient for the direct process according to the detailed balance relation (3).

### 3. Application to barium-hydrogen ionic collisions

In this section, the simplified model is applied for estimating rate coefficients of neutralization, ion-pair formation, and excitation and de-excitation processes in barium-hydrogen ionic collisions ( $Z = 1$ ). To the best of our knowledge no barium-hydrogen collision rates have been published.

Step 1: determining a ground ionic  $Ba^{2+} + H^-$  (diabatic) molecular state symmetry. For barium-hydrogen collisions, the ground ionic  $Ba^{2+}(5p^6 \ ^1S) + H^-(1s^2 \ ^1S)$  molecular state has the only symmetry,  $BaH^+(\ ^1\Sigma^+)$ . In this case, each sum in Eqs. (1) and (2) only has the term with  $\Lambda = 0$  and total spin  $S = 0$ .

Step 2: determining the barium ionic states to be treated and the corresponding electronic bound energies. It is necessary to determine barium-ion states, which (i) create  $BaH^+(\ ^1\Sigma^+)$  molecular states and (ii) correspond to single-electron transitions to the ground ionic molecular state. Only the ionic states with electronic bound energies that have values  $E_j < -1.3$  eV are taken into account; above this energy the rate coefficients are negligibly small along with states that correspond to multielectron transitions into the ground ionic molecular state. These barium ionic states with the corresponding scattering channels, electronic bound energies, and statistical probabilities are collected in Table 1.

Step 3: determining reduced rate coefficients.

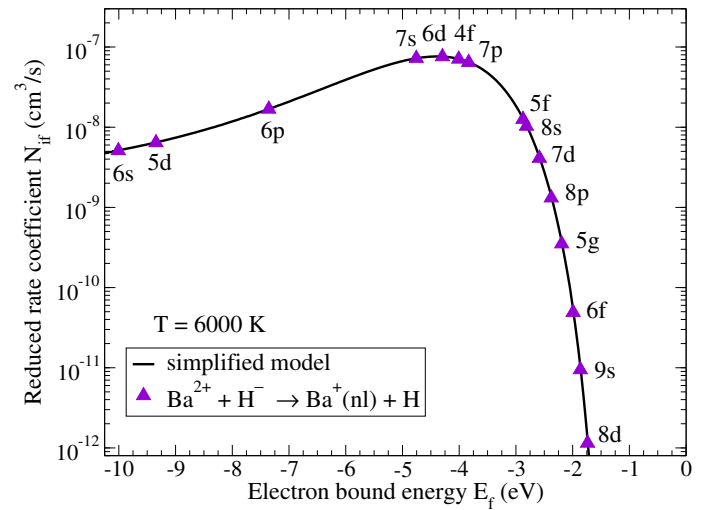
Step 3a. In order to estimate rate coefficients for a neutralization process, a reduced rate  $N_{if}(T; E_f)$  should be taken at a given temperature as a function of a final-state electronic bound energy  $E_f$ . At  $T = 6000$  K this function is plotted in Fig. 2 and shown again in Fig. 4 by solid lines. The reduced rate coefficients for particular neutralization processes in  $Ba^{2+} + H^-$  collisions are determined by the values of the function  $N_{if}(T; E_f)$  at the particular final electronic bound energies  $E_f$  from Table 1; see symbols in Fig. 4. For example, the final state  $Ba^+(6d \ ^2D)$  has the electronic bound energy  $E_f = -4.29573$  eV.

The corresponding reduced rate coefficient for the neutralization process  $Ba^{2+} + H^- \rightarrow Ba^+(6d \ ^2D) + H$  is equal to  $N_{if}(T = 6000 \text{ K}, E_f = -4.29573 \text{ eV}) = 7.59 \times 10^{-8} \text{ cm}^3/\text{s}$  (see Fig. 4). This rate coefficient has the highest value in these collisions.

Step 3b. In order to estimate rate coefficients for de-excitation and excitation processes, a reduced rate  $D_{if}(T; E_i, E_f)$  should be taken at a given temperature as a 2D function of the initial- and final-state electronic bound energies. At  $T = 6000$  K this function is plotted in Fig. 3. The reduced rate coefficients for particular excitation and de-excitation processes  $Ba^+(i) + H \rightarrow Ba^+(f) + H$  at a given temperature can first be determined as a cut of the 2D surface  $D_{if}(T; E_i, E_f)$  at an initial bound energy  $E_i$ , and then by taking particular values from this cut of  $D_{if}$  at the

**Table 1.** Scattering channels correlated to  $BaH^+(\ ^1\Sigma^+)$  molecular states, their statistical probabilities  $p_j^{\text{stat}}$  and the asymptotic energies equal to the electronic bound energies  $E_j$  ( $\bar{J}$  averaged experimental values taken from NIST, Kramida et al. 2016) with respect to the ionization limit  $Ba^{2+}(^1S) + H(1s \ ^2S)$ .

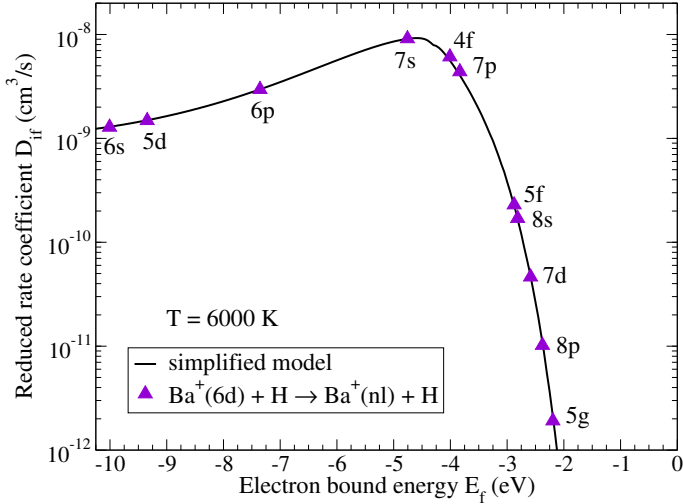
$j$	Scattering channels	Asymptotic energies = bound energies $E_j$ (eV)	$p_j^{\text{stat}}$
1	$Ba^+(6s \ ^2S) + H(1s \ ^2S)$	-10.0080	1/4
2	$Ba^+(5d \ ^2D) + H(1s \ ^2S)$	-9.34416	1/20
3	$Ba^+(6p \ ^2P) + H(1s \ ^2S)$	-7.35615	1/12
4	$Ba^+(7s \ ^2S) + H(1s \ ^2S)$	-4.75665	1/4
5	$Ba^+(6d \ ^2D) + H(1s \ ^2S)$	-4.29573	1/20
6	$Ba^+(4f \ ^2F) + H(1s \ ^2S)$	-4.00879	1/28
7	$Ba^+(7p \ ^2P) + H(1s \ ^2S)$	-3.83309	1/12
8	$Ba^+(5f \ ^2F) + H(1s \ ^2S)$	-2.87539	1/28
9	$Ba^+(8s \ ^2S) + H(1s \ ^2S)$	-2.81381	1/4
10	$Ba^+(7d \ ^2D) + H(1s \ ^2S)$	-2.58669	1/20
11	$Ba^+(8p \ ^2P) + H(1s \ ^2S)$	-2.37789	1/12
12	$Ba^+(5g \ ^2G) + H(1s \ ^2S)$	-2.19370	1/36
13	$Ba^+(6f \ ^2F) + H(1s \ ^2S)$	-1.99196	1/28
14	$Ba^+(9s \ ^2S) + H(1s \ ^2S)$	-1.86429	1/4
15	$Ba^+(8d \ ^2D) + H(1s \ ^2S)$	-1.73768	1/20
16	$Ba^+(9p \ ^2P) + H(1s \ ^2S)$	-1.62363	1/12
17	$Ba^+(6g \ ^2G) + H(1s \ ^2S)$	-1.52427	1/36
18	$Ba^+(7f \ ^2F) + H(1s \ ^2S)$	-1.42341	1/28
19	$Ba^+(10s \ ^2S) + H(1s \ ^2S)$	-1.32732	1/4
ionic	$Ba^{2+}(^1S) + H^-(1s^2 \ ^1S)$	-0.754	1



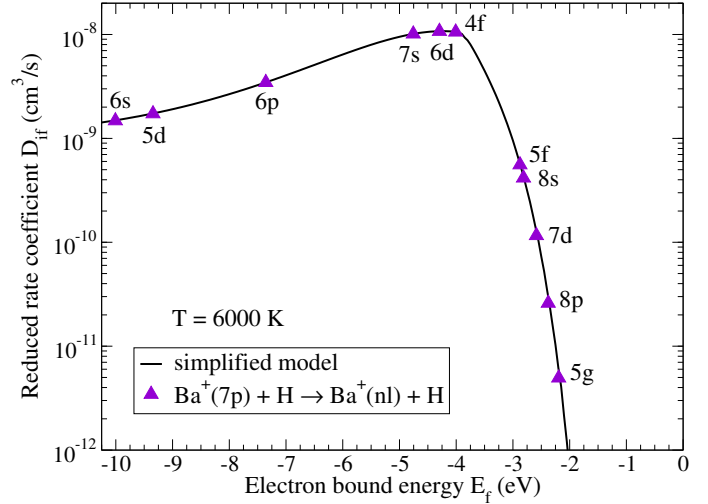
**Fig. 4.** General dependence of neutralization reduced rate coefficient  $N_{if}$  (solid line) on a final bound energy  $E_f$  and the particular reduced rate coefficients for  $Ba^{2+} + H^- \rightarrow Ba^+(f) + H$  processes (symbols) obtained by means of the present simplified model at  $T = 6000$  K.

final bound energies  $E_f$  (see Table 1). Examples of the excitation and de-excitation processes in barium-hydrogen ionic collisions are shown in Figs. 5–7 for the initial states  $i = 5–7$ .

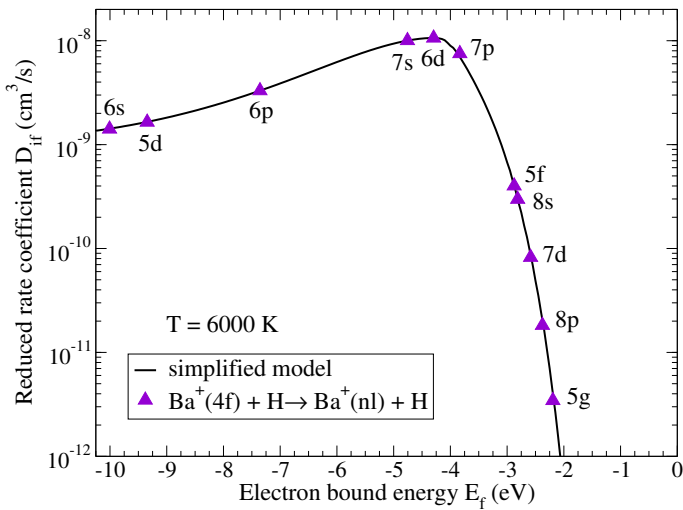
Step 4: estimating rate coefficients. Since the statistical probability  $p_{\text{ionic}}^{\text{stat}}$  for the ionic channel is presently equal to 1, the rate coefficients of the neutralization processes  $K_{if}(T)$  coincide with the corresponding reduced rate coefficients  $N_{if}$ , see Eq. (1). Rate coefficients for the ion-pair formation processes are calculated from the neutralization rates by the detailed balance Eq. (3).



**Fig. 5.** Cut of de-excitation/excitation reduced rate coefficient  $D_{if}(E_i, E_f)$  for particular de-excitation and excitation processes  $\text{Ba}^+(6d) + \text{H} \rightarrow \text{Ba}^+(f) + \text{H}$  for the initial bound energy  $E_i = E_5$  as a function of a final bound energy  $E_f$  (solid line) and the particular reduced rate coefficients for the same processes (symbols) obtained by means of the present simplified model at  $T = 6000$  K.



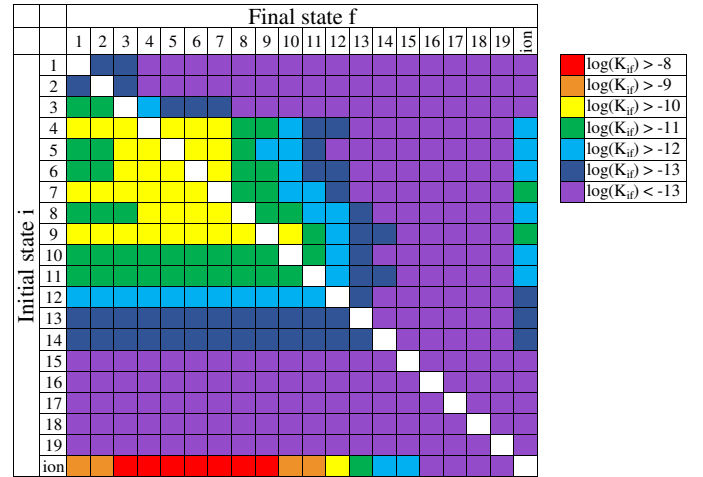
**Fig. 7.** Cut of de-excitation/excitation reduced rate coefficient  $D_{if}(E_i, E_f)$  for particular de-excitation and excitation processes  $\text{Ba}^+(7p) + \text{H} \rightarrow \text{Ba}^+(f) + \text{H}$  for the initial bound energy  $E_i = E_7$  as a function of a final bound energy  $E_f$  (solid line) and the particular reduced rate coefficients for the same processes (symbols) obtained by means of the present simplified model at  $T = 6000$  K.



**Fig. 6.** Cut of de-excitation/excitation reduced rate coefficient  $D_{if}(E_i, E_f)$  for particular de-excitation and excitation processes  $\text{Ba}^+(4f) + \text{H} \rightarrow \text{Ba}^+(f) + \text{H}$  for the initial bound energy  $E_i = E_6$  as a function of a final bound energy  $E_f$  (solid line) and the particular reduced rate coefficients for the same processes (symbols) obtained by means of the present simplified model at  $T = 6000$  K.

The rate coefficients  $K_{if}(T)$  for the de-excitation processes are calculated from the reduced rate coefficients  $D_{if}$  by multiplying the latter by the statistical probability  $p_i^{\text{stat}}$ ; see Eq. (2). Although rate coefficients  $K_{if}(T)$  for excitation processes can be calculated directly from the reduced rate coefficients  $D_{if}$ , it is more practical first to calculate the rate coefficients for the de-excitation processes and then to compute  $K_{if}(T)$  for excitation processes from the rate coefficients for the de-excitation processes using the detailed balance Eq. (3).

The rate coefficients  $K_{if}(T)$  for all possible processes in barium-hydrogen ionic collisions are estimated by the described simplified model and presented as the supplementary material for the temperature range  $T = 1000\text{--}10\,000$  K. The graphical representation of the calculated rate coefficients in



**Fig. 8.** Graphical representation of the rate coefficients in barium-hydrogen ionic collisions obtained by means of the simplified model at  $T = 6000$  K.

barium-hydrogen ionic collisions at  $T = 6000$  K is presented in Fig. 8. The high-valued rate coefficients  $K_{if}(T)$  are shown in Table 2 for the temperatures  $T = 2000, 6000, 10\,000$  K. It is seen that the highest values of the rate coefficients correspond to the neutralization processes into the  $\text{Ba}^+(6p) - \text{Ba}^+(8s)$  states and the moderate values correspond to the neutralization and the (de-)excitation processes from and to these states and the states around them; see Fig. 8 and Table 2, in agreement with the general rules discussed above.

#### 4. Conclusions

The simplified model is derived and described in detail in the present paper to estimate rate coefficients of inelastic processes in low-energy collisions of hydrogen atoms and negative ions with atoms and positive ions of other chemical elements; i.e.,  $\text{A}^{(Z+1)+} + \text{H}^-$  and  $\text{A}^{Z+}(j) + \text{H}$  collisions,  $Z = 0, 1, \dots$ . The main goal of the model is to estimate rate coefficients with high and

**Table 2.** Rate coefficients, in units of  $\text{cm}^3/\text{s}$ , for selected temperatures in the range  $T = 2000\text{--}10\,000$  K for the excitation, de-excitation, ion-pair formation, and mutual neutralization processes in barium-hydrogen ionic collisions.

Initial state	Final state												$i$
	1	2	3	4	5	6	7	8	9	10	11	12	
$T = 2000$ K													
1	—	1.23E-14	1.06E-17	1.55E-23	1.32E-24	2.82E-25	1.09E-25	3.98E-28	2.56E-28	4.13E-29	5.44E-30	6.34E-31	9.74E-33
2	1.15E-13	—	7.96E-17	1.62E-22	1.39E-23	3.01E-24	1.17E-24	4.18E-27	2.68E-27	4.24E-28	5.52E-29	6.37E-30	1.15E-31
3	1.70E-11	1.36E-11	—	4.66E-17	4.24E-18	9.33E-19	3.64E-19	1.10E-21	6.88E-22	1.00E-22	1.23E-23	1.35E-24	5.10E-26
4	2.65E-10	2.94E-10	4.97E-10	—	1.18E-10	2.64E-11	9.99E-12	1.91E-14	1.15E-14	1.52E-15	1.74E-16	1.81E-17	2.38E-18
5	6.54E-11	7.34E-11	1.31E-10	3.42E-10	—	7.97E-11	3.02E-11	5.46E-14	3.31E-14	4.39E-15	5.07E-16	5.36E-17	7.27E-18
6	5.29E-11	5.98E-11	1.09E-10	2.89E-10	3.01E-10	—	1.12E-10	1.98E-13	1.20E-13	1.62E-14	1.89E-15	2.03E-16	2.57E-17
7	1.32E-10	1.50E-10	2.75E-10	7.07E-10	7.36E-10	7.27E-10	—	1.22E-12	7.46E-13	1.02E-13	1.21E-14	1.32E-15	1.51E-16
8	5.35E-11	5.97E-11	9.22E-11	1.50E-10	1.48E-10	1.42E-10	1.36E-10	—	4.75E-11	6.79E-12	9.63E-13	1.25E-13	3.28E-15
9	3.45E-10	3.83E-10	5.76E-10	9.06E-10	8.97E-10	8.63E-10	8.28E-10	4.75E-10	—	6.33E-11	9.14E-12	1.21E-12	2.69E-14
10	4.15E-11	4.52E-11	6.29E-11	8.92E-11	8.89E-11	8.68E-11	8.44E-11	5.07E-11	4.73E-11	—	5.20E-12	7.51E-13	7.94E-15
11	3.06E-11	3.30E-11	4.32E-11	5.72E-11	5.75E-11	5.69E-11	5.60E-11	4.03E-11	3.82E-11	2.91E-11	—	3.09E-12	1.42E-14
12	3.46E-12	3.69E-12	4.59E-12	5.79E-12	5.90E-12	5.93E-12	5.93E-12	5.09E-12	4.92E-12	4.08E-12	3.00E-12	—	3.64E-15
i	8.11E-09	1.02E-08	2.65E-08	1.16E-07	1.22E-07	1.14E-07	1.04E-07	2.03E-08	1.66E-08	6.59E-09	2.10E-09	5.55E-10	—
$T = 6000$ K													
1	—	9.87E-13	3.27E-13	1.03E-14	5.10E-15	3.23E-15	2.41E-15	2.51E-16	1.97E-16	6.57E-17	1.66E-17	3.39E-18	2.15E-17
2	7.12E-13	—	2.13E-13	8.52E-15	4.27E-15	2.71E-15	2.03E-15	2.05E-16	1.60E-16	5.25E-17	1.31E-17	2.65E-18	1.96E-17
3	1.84E-11	1.66E-11	—	1.27E-12	6.63E-13	4.25E-13	3.16E-13	2.58E-14	1.97E-14	5.96E-15	1.40E-15	2.71E-16	3.99E-15
4	2.66E-10	3.04E-10	5.83E-10	—	9.34E-10	5.91E-10	4.24E-10	2.24E-11	1.66E-11	4.52E-12	9.92E-13	1.84E-13	7.87E-12
5	6.41E-11	7.43E-11	1.48E-10	4.55E-10	—	3.05E-10	2.19E-10	1.15E-11	8.50E-12	2.32E-12	5.11E-13	9.55E-14	4.02E-12
6	5.05E-11	5.88E-11	1.18E-10	3.58E-10	3.79E-10	—	2.68E-10	1.43E-11	1.07E-11	2.94E-12	6.52E-13	1.23E-13	4.67E-12
7	1.23E-10	1.44E-10	2.88E-10	8.43E-10	8.94E-10	8.80E-10	—	4.64E-11	3.46E-11	9.68E-12	2.16E-12	4.12E-13	1.39E-11
8	3.51E-11	3.96E-11	6.42E-11	1.22E-10	1.28E-10	1.28E-10	1.27E-10	—	6.33E-11	2.10E-11	5.54E-12	1.18E-12	7.41E-12
9	2.17E-10	2.44E-10	3.86E-10	7.11E-10	7.47E-10	7.52E-10	7.46E-10	5.00E-10	—	1.57E-10	4.26E-11	9.23E-12	4.80E-11
10	2.25E-11	2.49E-11	3.63E-11	6.01E-11	6.33E-11	6.44E-11	6.47E-11	5.14E-11	4.87E-11	—	1.12E-11	2.66E-12	5.93E-12
11	1.42E-11	1.55E-11	2.13E-11	3.29E-11	3.47E-11	3.57E-11	3.61E-11	3.38E-11	3.30E-11	2.80E-11	—	5.57E-12	4.74E-12
12	1.38E-12	1.49E-12	1.96E-12	2.91E-12	3.09E-12	3.21E-12	3.27E-12	3.44E-12	3.40E-12	3.16E-12	2.65E-12	—	6.03E-13
i	5.11E-09	6.42E-09	1.68E-08	7.24E-08	7.59E-08	7.08E-08	6.44E-08	1.26E-08	1.03E-08	4.11E-09	1.31E-09	3.51E-10	—
$T = 10\,000$ K													
1	—	4.60E-12	3.15E-12	5.98E-13	4.04E-13	3.08E-13	2.56E-13	4.54E-14	3.67E-14	1.37E-14	3.85E-15	8.57E-16	2.33E-14
2	1.99E-12	—	1.35E-12	3.02E-13	2.06E-13	1.57E-13	1.31E-13	2.22E-14	1.79E-14	6.57E-15	1.82E-15	4.02E-16	1.27E-14
3	2.28E-11	2.26E-11	—	1.04E-11	7.23E-12	5.50E-12	4.52E-12	6.09E-13	4.78E-13	1.62E-13	4.24E-14	8.99E-15	5.59E-13
4	2.65E-10	3.09E-10	6.37E-10	—	1.48E-09	1.09E-09	8.64E-10	7.49E-11	5.71E-11	1.74E-11	4.24E-12	8.62E-13	1.45E-10
5	6.12E-11	7.20E-11	1.51E-10	5.06E-10	—	4.02E-10	3.19E-10	2.75E-11	2.09E-11	6.38E-12	1.55E-12	3.17E-13	5.15E-11
6	4.65E-11	5.48E-11	1.15E-10	3.72E-10	4.01E-10	—	3.16E-10	2.80E-11	2.14E-11	6.57E-12	1.60E-12	3.29E-13	4.77E-11
7	1.11E-10	1.30E-10	2.70E-10	8.41E-10	9.09E-10	9.03E-10	—	8.02E-11	6.14E-11	1.90E-11	4.68E-12	9.67E-13	1.24E-10
8	2.55E-11	2.89E-11	4.73E-11	9.50E-11	1.02E-10	1.04E-10	1.04E-10	—	5.78E-11	2.16E-11	6.15E-12	1.39E-12	3.14E-11
9	1.55E-10	1.75E-10	2.79E-10	5.44E-10	5.84E-10	5.98E-10	6.01E-10	4.34E-10	—	1.55E-10	4.55E-11	1.04E-11	1.94E-10
10	1.51E-11	1.67E-11	2.47E-11	4.32E-11	4.64E-11	4.79E-11	4.85E-11	4.22E-11	4.04E-11	—	1.04E-11	2.60E-12	2.02E-11
11	8.98E-12	9.82E-12	1.37E-11	2.23E-11	2.39E-11	2.48E-11	2.53E-11	2.56E-11	2.52E-11	2.21E-11	—	4.82E-12	1.38E-11
12	8.26E-13	8.96E-13	1.20E-12	1.87E-12	2.02E-12	2.11E-12	2.16E-12	2.39E-12	2.38E-12	2.28E-12	1.99E-12	—	1.53E-12
i	4.31E-09	5.43E-09	1.43E-08	6.02E-08	6.27E-08	5.83E-08	5.30E-08	1.03E-08	8.46E-09	3.39E-09	1.09E-09	2.93E-10	—



moderate values; that is, the rates that are important for non-LTE stellar atmosphere modeling. The model is based on the main reaction mechanism of the processes under consideration, which is determined by nonadiabatic transitions in long-range regions created by ionic-covalent molecular-state interactions.

Within the simplified model, the rate coefficients are expressed via reduced rate coefficients that are different for neutralization and ion-pair formation processes  $A^{(Z+1)+} + H^- \rightleftharpoons A^{Z+}(f) + H$  and for excitation/de-excitation processes  $A^{Z+}(i) + H \rightarrow A^{Z+}(f) + H$ . It is shown that the reduced rate coefficients for neutralization and ion-pair formation processes depend on a single electronic bound energy of an atomic/ionic state  $A^{Z+}(f)$ , which correlates to a corresponding covalent molecular state, while the reduced rate coefficients for excitation/de-excitation processes depend on two bound energies: electronic bound energies for an initial and a final atomic/ionic states. The reduced rate coefficients are calculated and tabulated for the case  $Z = 0$  in Paper I, while these coefficients are calculated for cases  $Z = 1, 2$  in the present paper. Optimal windows for neutralization and ion-pair formation and for excitation/de-excitation processes are determined as well.

The simplified method does not have any adjustable parameters. Moreover, one does not need to perform any complicated calculations; all calculations of reduced rate coefficients have been accomplished and tabulated in Paper I and in the present paper, and finally the rate coefficients can be estimated by the simple Eqs. (1)–(3). Without any additional calculation, the method indicates which processes have high and moderate rate coefficients, and hence are expected to be important for non-LTE stellar atmosphere modeling.

Furthermore, the simplified method helps in understanding a general distribution of inelastic rate coefficients in collisions of various chemical elements with hydrogen. In particular, the method selects atomic/ionic states that are efficiently involved in the inelastic H-collision processes. This is carried out by determining the optimal windows of atomic/ionic states; that is, by determining the electronic bound energy intervals for atomic/ionic states whose participation leads to high and moderate rate coefficients. It is shown that these intervals are the same for all chemical elements. For  $Z = 0$ , they are located in the vicinity of the electronic bound energy  $-2$  eV, for  $Z = 1$  around  $-4.4$  eV, and for  $Z = 2$  around  $-8.2$  eV.

The simplified method allows rate coefficients to be estimated for neutralization, ion-pair formation, excitation, and de-excitation processes in collisions of hydrogen with many chemical elements. In the present paper, the simplified model is applied

to barium-hydrogen ionic collisions,  $Z = 1$ . The rate coefficients for the most important neutralization, ion-pair formation, excitation, and de-excitation processes are estimated and presented at the CDS.

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