Inelastic Processes in Nickel–Hydrogen Collisions

Yaroslav V. Voronov®, Svetlana A. Yakovleva®, and Andrey K. Belyaev®

Department of Theoretical Physics and Astronomy, Herzen University, St. Petersburg 191186, Russia; andrey.k.belyaev@gmail.com

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Abstract

The cross sections and rate coefficients for inelastic processes in low-energy collisions of nickel atoms and positive ions with hydrogen atoms and negative ions are calculated for the collisional energy range $10^{-3}$–100 eV and for the temperature range 1000–10,000 K. 74 covalent and three ionic states correlated to 11 molecular symmetries are considered. 3380 partial inelastic processes are treated in total. The study of nickel–hydrogen collisions is performed by the quantum model methods within the Born–Oppenheimer formalism. The electronic structure of the collisional quasimolecule is calculated by the semiempirical asymptotic method for each considered molecular symmetry. For nuclear dynamic calculations the simplified method in combination with the Landau–Zener model is used. Nuclear dynamics within each considered symmetry is treated separately, and the total rate coefficients for each inelastic process have been summed over all symmetries. The largest values of the rate coefficients (exceeding $10^{-8}$ cm$^3$ s$^{-1}$) correspond to the mutual neutralization processes in collisions Ni$^+$($3d^{9}2D$) + H$^+$ (1$S^{2}$1$S$) (the ground ionic state being the initial state), as well as in Ni$^+$($3d^44s^24F$) + H$^+$ (1$S^{2}$1$S$) (the first excited and the second excited ionic states being the initial states) collisions. At the temperature of 6000 K, the rate coefficients with large magnitudes have the values from the ranges $(1.35–5.87) \times 10^{-8}$ cm$^3$ s$^{-1}$ and $(1.02–6.77) \times 10^{-8}$ cm$^3$ s$^{-1}$, respectively. The calculated rate coefficients with large and moderate values are important for non–local thermodynamic equilibrium stellar atmosphere modeling.

Unified Astronomy Thesaurus concepts: Collision processes (2065)

Supporting material: tar.gz file

1. Introduction

Stellar atmosphere modeling beyond the local thermodynamic equilibrium (LTE) approximation, that is, within the so-called non-LTE, allows one to obtain important information not only qualitatively but also quantitatively about the composition of stars. However, this is correct when information about inelastic processes in stellar atmospheres is accurate enough. First of all, this is relevant to collisions of heavy particles with hydrogen atoms and ions because hydrogen is the most abundant element in the universe. For each element, investigations are carried out individually. For example, iron-peak elements are of fundamental interest.

Nickel, as a representative of the Fe group, is one of the most important chemical elements in modern astrophysics. The decay radioisotope $^{56}$Ni to $^{56}$Fe shapes the light curves of supernovae Ia (SN Ia) systems and thus, the amount of Ni is critical for understanding the progenitor channels and properties of SN Ia, that have been used as standardizable “candles” in observational cosmology (see, e.g., Phillips 1993; Riess et al. 1996; Scalzo et al. 2014; Abbott et al. 2019). For the same reason, abundances of Ni in stars are commonly used to disentangle the role of different SN Ia types in Galaxy evolution (see, e.g., Kobayashi et al. 2020a; Sanders et al. 2021). In particular, the role of sub-Chandrasekhar (sub-Ch) mass SN Ia in Galactic chemical evolution (GCE) has been discussed extensively (see, e.g., Seitenzahl & Townsley 2017; Eitner et al. 2020). It shall be noted, however, that standard GCE models underproduce [Ni/Fe] below metallicities of $\sim$–1 in the Galactic disk and halo (see, e.g., Kobayashi et al. 2020b; Palla 2021). More recently, attempts were made to constrain the SN Ia physics in dwarf Spheroidal galaxies (see, e.g., Kirby et al. 2019; de los Reyes et al. 2020). Complementary studies aim to investigate the sub-Ch to Ch SN Ia fractions using Ni/Fe ratios inferred from the analysis of late-type SN Ia spectra (see, e.g., Flörs et al. 2020; Siebert et al. 2020).

Additionally, the solar abundance of Ni is still debated (Caffau et al. 2011 but Asplund et al. 2021), and this has consequences for constraining the solar metallicity, which is important for models of the solar structure and evolution (so-called SSM; e.g., Serenelli et al. 2011; Buldgen et al. 2019). The main uncertainty with modeling the critical forbidden OI line at 6300.30 Å in the solar spectrum is associated with its blend—the weak line of Ni at 6300.34 Å. Therefore the oxygen abundance of the Sun inferred from this otherwise rather reliable [O I] line is only as good as our understanding of the abundance of Ni in the solar photosphere.

So far, most studies of the Ni abundances in stellar photopsheres adopted the LTE assumption. Only very few studies modeled Ni in the full non-LTE framework (Bruls 1993; Ding et al. 2002; Vieytes & Fontenla 2013), and Bergemann et al. (2021) for the first time used a detailed model of Ni in the 3D non-LTE analysis of the solar O + Ni spectral feature. Their Ni model was based on the classical Darwin recipe to describe the processes in collisions between NiI and H atoms.

Therefore, in this work we attempt to remove one of the critical uncertainties in the non-LTE modeling of Ni abundances in stellar spectra, by performing detailed quantum-mechanical calculations of the inelastic processes in Ni$^+$ + H and Ni$^+$ + H$^+$ collisions. The point is that, in the past, rate coefficients of the inelastic H-collision processes were estimated by the Darwin formula. The comparison of the results obtained with the Darwin formula and ones with the accurate quantum calculations has been published (by figures) for inelastic processes in the following collisions: Na$^+$ + H and Na$^+$ + H$^+$ (Barklem et al. 2011), Mg$^+$ + H and Mg$^+$ + H$^+$ (Barklem et al. 2012), Mn$^+$ + H and Mn$^+$ + H$^+$ (Bergemann et al. 2019), Fe,
Fe$^+$ + H, and Fe$^+$, Fe$^{2+}$ + H$^-$ (Mashonkina et al. 2019). This comparison shows that some Drawin rate coefficients are overestimated by several orders of magnitude (for optically allowed transitions), and some others are underestimated also by several orders of magnitude (for optically forbidden transitions). In particular, the Drawin formula gives zero values for charge-transfer processes that usually have the highest rate coefficients. Thus, the Drawin formula does not provide reliable results (see Barklem et al. 2011 for details), and it should be replaced by physically reliable quantum calculations, which provide correct H-collisional data. For nickel, this is accomplished in the present work.

2. Brief Theory

The present study of the inelastic processes in nickel–hydrogen collisions continues systematical investigations of the state-to-state processes in collisions of hydrogen atoms and anions with atoms and cations of various chemical elements of astrophysical importance. The studies include different quantum approaches from rigorous quantum methods (see Belyaev et al. 2010, 2012, 2014, 2019a, and references therein) to different models (see Belyaev 2013; Belyaev et al. 2017, 2018; Belyaev & Yakovleva 2017a; Belyaev & Voronov 2018; Belyaev et al. 2019b; Belyaev & Voronov 2021, and references therein). It has been shown that, for reliable non-LTE modeling, the critical uncertainties are associated with inelastic H-collision processes with large and moderate rate coefficients. In order to estimate such rate coefficients, several quantum models have been proposed and applied for calculating both the electronic structure and nonadiabatic nuclear dynamics. Comparison of the model results with full quantum calculations (see above for references) and with available experimental data (see, e.g., Launoy et al. 2019; Belyaev & Voronov 2021 for the mutual neutralization processes in Li$^+$ + H$^-$ collisions) shows good agreement. For this reason, the quantum models are used in the present study for estimating the large- and moderate-valued rate coefficients of inelastic processes in nickel–hydrogen collisions.

Concerning the electronic structure, even the estimates show that the NiH structure is complicated. For this reason, the electronic structures of all states, ionic and covalent, of a NiH molecule are estimated by means of the quantum asymptotic semiempirical method (Belyaev 2013). The nonadiabatic nuclear dynamics were then studied by means of a simplified model (Belyaev & Yakovleva 2017a, 2017b).

The background of the simplified model is the following. Several quantum calculations (see, e.g., Belyaev et al. 2012) have shown that the dominant mechanism of the inelastic processes in collisions with hydrogen corresponds to long-range ionic–covalent interactions. The asymptotic diabatic potentials are mainly determined by the Coulomb potentials for the ionic A$^+$ + H$^-$ states and by flat potentials for the covalent A + H states. The off-diagonal matrix elements of the long-range ionic–covalent interactions are evaluated by the semi-empirical Olson–Smith–Bauer formula (Olson et al. 1971). All these allow one to determine the locations and parameters of nonadiabatic regions.

Belyaev & Yakovleva (2017a) introduced the concept of the reduced cross sections and the reduced rate coefficients; see Equations (1)–(5) of that paper. The standard rate coefficients are determined via the reduced rate coefficients as follows. The (standard) rate coefficient of an inelastic state-to-state collisional process is equal to the sum over molecular state symmetries created by both the initial and final scattering channels; each term in this sum is a product of a statistical probability $p_{\text{stat}}$ for a treated initial molecular state, and a reduced rate coefficient for the treated transition. It is easy to see that, if the nonadiabatic nuclear dynamics for a treated transition is identical in all molecular states corresponding to the initial scattering channel and the final scattering channel has all these molecular states of these symmetries, then the (standard) rate coefficient is equal to the corresponding reduced rate coefficient; otherwise, the (standard) rate coefficient is lower than the reduced rate coefficient.

It was shown by Belyaev & Yakovleva (2017a, 2017b) that, in the case that the nonadiabatic region information is determined as described above, then the nonadiabatic transition probabilities, reduced partial cross sections, and reduced partial rate coefficients for the processes of the mutual neutralization and their inverse processes—ion-pair formation are determined by a single binding energy of a corresponding covalent scattering channel, while for excitation and de-excitation processes, the corresponding reduced values are determined by two binding energies—of the initial and final scattering channels. The reduced rate coefficients were tabulated as functions of the corresponding binding energies (Belyaev & Yakovleva 2017a, 2017b). The state-to-state transition probabilities were calculated within the two-state approximation by the Landau–Zener formula (Landau 1932a, 1932b; Zener 1932). Finally, the complete rate coefficients, defined by the standard formulas (see, e.g., Yakovleva et al. 2016; Belyaev & Yakovleva 2017a), can be written via products of the tabulated reduced rate coefficients and the statistical probabilities of the corresponding initial channel, as defined above. The products should be summed over the molecular state symmetries, in which the transitions occur. Thus, knowing the dependences of the reduced rate coefficients on the corresponding binding energies (see Belyaev & Yakovleva 2017a, 2017b, for details) allows one to estimate the partial state-to-state rate coefficients by means of the simplified model without additional calculations.

The present study considers 77 scattering channels: 74 channels asymptotically correlate to covalent molecular states Ni (1$^3\Sigma$–$^1\Sigma$), 3 channels to the ionic states Ni$^+$ (3$^3D$) + H$^-$ and Ni$^+$ (3$^3D$ 4$^3S$) + H$^-$). The simplified model used in the present work treats the inelastic processes due to one-electron transitions only. The results are discussed below.

3. Nickel–Hydrogen Collision Processes

Ionic molecular states have different electronic configurations, and that is why two sets of calculations are performed: one-electron-transition processes due to the interaction of the covalent states with the Ni$^+$ (3$^3D$) + H$^-$ ionic state and one-electron-transition processes due to the interaction with Ni$^+$ (3$^3D$ 4$^3S$) + H$^-$ ionic states.

The molecular states Ni (3$^3D$ 3$^3S$) + H and Ni$^+$ (3$^3D$) + H$^-$, which are included in the first set of the rate coefficients calculations, are collected in Table 1 together with the asymptotic energy values and statistical probabilities $p_{\text{stat}}$ for populations of the molecular states. The Ni$^+$ (3$^3D$) + H$^-$ scattering channel produces molecular states of $^2\Sigma$+, $^2\Pi$, and $^2\Delta$ symmetries, so only covalent states of the same molecular symmetries are taken into account in the present study.

The second set of calculations includes the scattering channels Ni (3$^3D$ 4$^3S$) + H and Ni$^+$ (3$^3D$) + H$^-$). Their asymptotic energies and statistical probabilities $p_{\text{stat}}$ are collected in Table 2. The ionic scattering channel Ni$^+$ (3$^3D$ 4$^3S$) + H$^-$ produces molecular states of $^4\Sigma$–, $^4\Pi$, $^4\Delta$ and $^4\Phi$ molecular symmetries, while the ionic scattering
channel $Ni^+(3d^8 4s^2 F) + H^- \rightarrow \Sigma^-$ produces $\Sigma^-$, $2\Pi$, $2\Delta$, and $2\Phi$ molecular states. The covalent molecular states of these symmetries are included in the second set of calculations. The rate coefficients of the inelastic processes are calculated within each molecular symmetry separately and then summed over the initial and final channels of the process.

The scattering channels of Ni + H that do not produce molecular states of the same symmetries as any of ionic states are not included into a consideration, as well as the scattering channels that form nonadiabatic regions at large internuclear distances because the transition probabilities are negligibly small.

Figure 1 shows a graphical representation of all calculated rate coefficients for inelastic processes in collisions of $Ni^+(3d^{2}D) + H^{-}(1s^2 S)$ and $Ni(3d^9nl 1.5 L) + H(1s^2 S)$ at the temperature of $T = 6000$ K. The complete data calculated in the present work, which are the rate coefficients for all inelastic transition processes between the scattering channels described above for the temperature range from 1000 to 10000 K, are collected as the supplementary material in the .tar.gz package. One can see that the rate coefficients with values exceeding $10^{-8}$ cm$^3$ s$^{-1}$ (red squares) correspond to the mutual neutralization processes with the following final states of the nickel atom: $Ni(3d^9l^2D5s 3D)$ with a value of $3.54 \times 10^{-8}$ cm$^3$ s$^{-1}$, $Ni(3d^9l^2D5s 3D)$ with a value of $5.87 \times 10^{-8}$ cm$^3$ s$^{-1}$, $Ni(3d^9l^2D5p 3F)$ with a value of $1.42 \times 10^{-8}$ cm$^3$ s$^{-1}$, and $Ni(3d^9l^2D5p 3F)$ with a value of $1.35 \times 10^{-8}$ cm$^3$ s$^{-1}$. Rates with moderate values $10^{-12}$–$10^{-10}$ cm$^3$ s$^{-1}$ (orange, yellow, green, and light blue squares) correspond to other neutralization processes, ion-pair formation, excitation, and de-excitation processes.

A graphical representation of all calculated rate coefficients for inelastic processes in collisions of $Ni^+(3d^8 4s^2 F) + H^{-}(1s^2 S)$ and $Ni(3d^9nl 1.5 L) + H(1s^2 S)$ is shown in Figure 2 for a temperature of $T = 6000$ K. It is worth noting that the processes $Ni^+(3d^8 4s^2 F) + H^{-}(1s^2 S)$ and $Ni(3d^9nl 1.5 L) + H(1s^2 S)$ are treated separately since the corresponding molecular states have different multiplicities; the rate coefficients for the processes involving molecular states with both multiplicities (atomic states $Ni(L)$) are then summed. It can be seen that several neutralization processes from both ionic states $Ni^+(3d^8 4s^2 F) + H^{-}(1s^2 S)$ and $Ni^+(3d^8 4s^2 F) + H^{-}(1s^2 S)$ have values of rate coefficients exceeding $10^{-8}$ cm$^3$ s$^{-1}$. It should also be noted that the rate coefficients with moderate values (orange, yellow, green, and light blue squares) correspond to transitions between higher
excited states as compared to Figure 1. The reason for that is the following: the simplified model gives high and moderate values of the rate coefficients to the processes involving states with asymptotic energies in the “optimal window”1 that lies 2 eV lower than the ionization energy of an atom. In the case of the ground ionic state Ni+ (3d^6 2D), this “optimal window” is located around 5.64 eV, while for the first excited state Ni+ (3d^6 4s^2 F), it is located around 6.68 eV, and for the second excited ionic state Ni+ (3d^6 4s^2 F) around 7.32 eV. Thus, for different ionic scattering channels, the “optimal window” selects different final scattering channels.

Figure 3 shows the mutual neutralization rate coefficients for a temperature of T = 6000 K as a function of the excitation energy of the nickel atom for three sets of processes. The first panel corresponds to the processes with the ground ionic state being the initial channel, and the second panel for the processes with the first excited ionic state being the initial channel, and the third panel for the second excited ionic state being the initial channel (see Table 1), the second panel for the processes with the first excited ionic state being the initial channel, and the third panel for the second excited ionic state being the initial channel (see Table 2 for both). The reduced rate

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1 By an “optimal window”, we mean an atomic-binding-energy range such that scattering channels located into this range have large-valued rate coefficients.
Figure 1. Graphical representation of the rate coefficients (in cm$^3$ s$^{-1}$) for the partial excitation, de-excitation, mutual neutralization, and ion-pair formation processes in Ni ($3d^8nl^1l$) + H and Ni$^+$($3d^72D$) + H$^-$ collisions for a temperature of $T = 6000$ K. Initial and final state labels are presented in Table 1.

The rate coefficient with the lowest values (less than $10^{-12}$ cm$^3$ s$^{-1}$) is shown in Figure 3 with a solid line. The difference between the reduced rate coefficient and the one calculated in this study is due to the fact that some of the covalent states do not have all sets of the molecular symmetries as the ionic states. It is worth emphasizing that the ground ionic scattering channel has three molecular symmetries (see Table 1); each of the first and second excited ionic scattering channels has four molecular symmetries (see Table 2). Within the simplified model, the nonadiabatic nuclear dynamics are identical in each molecular symmetry for a treated scattering channel, and, hence, the reduced rate coefficients are equal to one another for each ionic scattering channel. That is why the reduced rate coefficient is plotted by a single curve instead of multiple coinciding curves in each panel of Figure 3, that is, for each ionic scattering channel treated. Moreover, as mentioned above, in cases when the final scattering channel has all molecular states of the treated symmetries, then the rate coefficient is equal to the corresponding reduced rate coefficient. Otherwise, the rate coefficient is lower than the corresponding reduced rate coefficient. This rule holds not only for the ground ionic state but also for the excited ionic states with a variation in the parameters (see, e.g., Figure 3).

Ultimately, all inelastic processes can be divided into three groups according to the values of their rate coefficients:

1. the rate coefficients with the largest values (exceeding $10^{-8}$ cm$^3$ s$^{-1}$; red squares in Figures 1, 2);
2. the rate coefficients with moderate values (between $10^{-12}$ and $10^{-8}$ cm$^3$ s$^{-1}$; orange, yellow, green and light blue squares in Figures 1, 2);
3. the rate coefficients with the lowest values (less than $10^{-12}$ cm$^3$ s$^{-1}$; blue squares in Figures 1, 2).

The first group includes several mutual neutralization processes: Ni$^+$(3d$^72D$) + H$^-$→Ni(3d$^8$5s$^1$D); Ni$^+$(3d$^8$5p$^1$3F) + H (j = 31 → j = 11–14 in Table 1) with values in the range of (1.35−5.8)$×10^{-8}$ cm$^3$ s$^{-1}$ at the temperature of $T = 6000$ K. Additionally, the mutual neutralization processes due to the transitions from the Ni$^+$(3d$^8$4s$^2$F) + H (1s$^2$5s) (j = 47) to the states j = 27, 31–33, 35–38, and 41 in Table 2 have values in the range of (1.02−6.77)$×10^{-8}$ cm$^3$ s$^{-1}$ at the temperature of $T = 6000$ K. Finally, the mutual neutralization due to the transitions from Ni$^+$(3d$^8$4s$^2$F) + H (1s$^2$5s) (j = 48) to the final states j = 33–35 and 39–44 in Table 2 have values in the range of (1.41−5.25)$×10^{-8}$ cm$^3$ s$^{-1}$.

The second group consists of excitation, de-excitation, ion-pair formation, and mutual neutralization processes that correspond to the transition between scattering channels that have asymptotic energies in the range of 5.3–6.3 eV (states j = 11–28 in Table 1) for the first set of calculated rate coefficients and scattering channels that have asymptotic energies in the range of 5.7–7.3 eV for the second set of calculated rate coefficients (states j = 24–48 in Table 2). These processes are shown by the orange, yellow, green, and light blue squares in Figure 1, 2. The processes from these two groups are likely to be important for astrophysical applications.

The third group consists mostly of the excitation processes but includes several de-excitation and ion-pair formation processes as well. The processes from this group mainly involve lower-lying states: 10 lowest states from the first set of calculations (see Table 1) and 16 lowest states from the second set of calculations (see Table 2).

4. Conclusion

In the present work, the inelastic processes in nickel–hydrogen collisions are studied for the first time using a simplified quantum model approach. The total number of considered scattering channels is 77 (74 covalent and 3 ionic). The total number of the investigated processes is 3380; those involving the ground ionic state, first excited ionic state, and second excited ionic state are 930, 1260, and 1190, respectively. The rate coefficient calculations can be divided into two sets:

1. Inelastic processes involving the ground ionic state of nickel Ni$^+$(3d$^72D$). These processes occur in three molecular symmetries: Σ$^+$, Π, and Δ. The rate coefficients are obtained as a sum of all considered molecular symmetries;
2. Inelastic processes involving the first excited ionic state of nickel Ni$^+$(3d$^8$4s$^2$F) occur in four molecular symmetries: Σ$^-$, Π, Δ, and Φ. Inelastic processes involving the second excited ionic state of nickel Ni$^+$(3d$^8$4s$^2$F) occur in molecular symmetries Σ$^-$, Π, Δ, and Φ. All calculations within these eight symmetries are treated separately, and the rate coefficients are obtained as a sum.

It is shown that the largest values (exceeding $10^{-8}$ cm$^3$ s$^{-1}$) of the rates correspond to several mutual neutralization processes. A number of excitation, de-excitation, ion-pair formation, and mutual neutralization processes have rate coefficients with moderate values ($10^{-8}$−$10^{-12}$ cm$^3$ s$^{-1}$); the majority of these processes involve transitions to nickel.
atomic states that have excitation energies in the range of 5.3–6.3 eV for the first set of calculations and 5.7–7.3 eV for the second set. These rate coefficients are expected to be important for the non-LTE stellar atmosphere modeling.

The simplified model has been applied to various inelastic processes in collisions of hydrogen with different chemical elements of astrophysical importance. Neutral and ionic collisions have been studied. The analysis of both the results

Figure 2. Graphical representation of the rate coefficients (in cm$^3$ s$^{-1}$) for the partial excitation, de-excitation, mutual neutralization, and ion-pair formation processes in Ni (3d$^8$ 4s $^1$S$^2$L) + H and Ni$^+$ (3d$^8$ 4s $^2$F) + H$^-$ collisions for a temperature of $T = 6000$ K. Initial and final state labels are presented in Table 2. The color legend is the same as in Figure 1.

Figure 3. Rate coefficients for mutual neutralization in nickel–hydrogen collisions (symbols) at $T = 6000$ K as a function of the excitation energy of Ni in the final state. Note the different reduced rate coefficient dependence (solid lines) for different initial ionic states Ni$^+$ + H$^-$. 

atomic states that have excitation energies in the range of 5.3–6.3 eV for the first set of calculations and 5.7–7.3 eV for the second set. These rate coefficients are expected to be important for the non-LTE stellar atmosphere modeling.

The simplified model has been applied to various inelastic processes in collisions of hydrogen with different chemical elements of astrophysical importance. Neutral and ionic collisions have been studied. The analysis of both the results
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and their applications to non-LTE modeling shows that rate coefficients with large values (from the first group) are estimated with a rather high accuracy (a few per cents) and are the most important for applications. Rate coefficients with moderate values (from the second group) are estimated within 1 order of magnitude and are also rather important for applications, while rate coefficients with low values are estimated with the lowest accuracy, but they are likely not important for astrophysical applications; nevertheless, it is useful to estimate them in order to know that they are low and negligible.

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ORCID iDs
Yaroslav V. Voronov @ https://orcid.org/0000-0002-4377-7827
Svetlana A. Yakovleva @ https://orcid.org/0000-0002-8889-7283
Andrey K. Belyaev @ https://orcid.org/0000-0001-8834-1456

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