Atomic data on inelastic processes in low-energy manganese-hydrogen collisions[★]

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ABSTRACT

Aims. The aim of this paper is to calculate cross sections and rate coefficients for inelastic processes in low-energy $\text{Mn} + \text{H}$ and $\text{Mn}^+ + \text{H}^-$ collisions, especially, for processes with high and moderate rate coefficients. These processes are required for non-local thermodynamic equilibrium (non-LTE) modeling of manganese spectra in cool stellar atmospheres, and in particular, for metal-poor stars.

Methods. The calculations of the cross sections and the rate coefficients were performed by means of the quantum model approach within the framework of the Born-Oppenheimer formalism, that is, the asymptotic semi-empirical method for the electronic MnH molecular structure calculation followed by the nonadiabatic nuclear dynamical calculation by means of the multichannel analytic formulas.

Results. The cross sections and the rate coefficients for low-energy inelastic processes in manganese-hydrogen collisions are calculated for all transitions between 21 low-lying covalent states and one ionic state. We show that the highest values of the cross sections and the rate coefficients correspond to the mutual neutralization processes into the final atomic states $\text{Mn}(3d^5 4s(^7S)5s\ e\ ^6S)$, $\text{Mn}(3d^5 4s(^7S)5p\ y\ ^8P^\circ)$, $\text{Mn}(3d^5 4s(^7S)5s\ e\ ^8S)$, $\text{Mn}(3d^5 4s(^7S)4d\ e\ ^8D)$ [the first group], the processes with the rate coefficients (at temperature $T = 6000\text{ K}$) of the values 4.38×10^{-8} , 2.72×10^{-8} , 1.98×10^{-8} , and $1.59 \times 10^{-8}\text{ cm}^3/\text{s}$, respectively, that is, with the rate coefficients exceeding $10^{-8}\text{ cm}^3/\text{s}$. The processes with moderate rate coefficients, that is, with values between 10^{-10} and $10^{-8}\text{ cm}^3/\text{s}$ include many excitation, de-excitation, mutual neutralization and ion-pair formation processes. In addition to other processes involving the atomic states from the first group, the processes from the second group include those involving the following atomic states: $\text{Mn}(3d^5(^6S)4s4p\ (^1P^\circ)\ y\ ^6P^\circ)$, $\text{Mn}(3d^5 4s(^7S)4d\ e\ ^6D)$, $\text{Mn}(3d^5 4s(^7S)5p\ w\ ^6P^\circ)$, $\text{Mn}(3d^5(^4P)4s4p\ (^3P^\circ)\ y\ ^6D^\circ)$, $\text{Mn}(3d^5(^4G)4s4p\ (^3P^\circ)\ y\ ^6F^\circ)$. The processes with the highest and moderate rate coefficients are expected to be important for non-LTE modeling of manganese spectra in stellar atmospheres.

Key words. atomic data – atomic processes – stars: abundances

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). Suffices it to say that non-LTE modeling of stellar atmospheres are of importance, in particular, for determining absolute and relative abundances of different 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 ones in collisions with hydrogen atoms and negative ions. It has been emphasized several times (see, e.g., [Asplund 2005](#); [Barklem 2016a](#)) that inelastic processes in collisions with hydrogen atoms and anions give the main uncertainty for non-LTE studies, especially in metal-poor stars.

The most accurate information about inelastic processes in low-energy collisions with hydrogen is that obtained by full quantum calculations. Recently, the markable progress has been

achieved in detailed quantum treatments of inelastic processes in collisions of different atoms and positive ions with hydrogen atoms and negative ions. The accurate quantum cross sections were calculated for transitions between many low-lying atomic and ionic states for Na, Li, Mg, He + H, as well as Na^+ , Li^+ , $\text{Mg}^+ + \text{H}^-$ collisions ([Belyaev et al. 1999, 2010, 2012](#); [Croft et al. 1999a,b](#); [Belyaev & Barklem 2003](#); [Guitou et al. 2015](#); [Belyaev 2015](#)) based on accurate ab initio ([Belyaev et al. 1999](#); [Guitou et al. 2010, 2015](#); [Belyaev 2015](#)) or pseudopotential ([Croft et al. 1999a](#); [Dickinson et al. 1999](#)) quantum-chemical data. The quantum cross sections were used for computing the inelastic rate coefficients ([Barklem et al. 2003, 2010, 2012](#); [Guitou et al. 2015](#)) and finally for the non-LTE stellar atmosphere modeling ([Barklem et al. 2003](#); [Lind et al. 2009, 2011](#); [Mashonkina 2013](#); [Osorio et al. 2015](#); [Osorio & Barklem 2016](#)).

Nevertheless, full quantum calculations are still time-consuming and, hence, rather seldom. For this reason, it was stated several times (see, e.g., [Asplund 2005](#); [Barklem et al. 2011](#)) that there is a strong demand in more approximate, but reliable model approaches¹. Two quantum model approaches

[★] Rate coefficients $K_{if}(T)$ for the excitation, de-excitation, mutual neutralization, and ion-pair formation processes in manganese-hydrogen collisions are only available at the CDS via anonymous ftp to cdsarc.u-strasbg.fr (130.79.128.5) or via <http://cdsarc.u-strasbg.fr/viz-bin/qcat?J/A+A/606/A106>

¹ Here we do not discuss the so-called Drawin formula, which is known to be unreliable, see ([Barklem et al. 2011](#)) for the critical analysis.

for nonadiabatic nuclear dynamics have been recently proposed and successfully applied: (i) the branching probability current method (Belyaev 2013a) and (ii) the multichannel model approach (Belyaev 1993; Belyaev et al. 2014b; Yakovleva et al. 2016). Both approaches are based on electronic structure calculations and the Landau-Zener model for nonadiabatic transitions. For electronic structure calculations, in addition to accurate ab initio methods, the following approximate methods have been used: the asymptotic method (Belyaev 2013a) and the Linear Combinations of Atomic Orbitals (LCAO) method (Grice & Herschbach 1974; Adelman & Herschbach 1977; Barklem 2016b). The quantum model approaches have been successfully applied to a number of low-energy inelastic processes in collisions with hydrogen: Al (Belyaev 2013a), Li, Mg, Si (Belyaev et al. 2014b), Cs (Belyaev et al. 2014a), Be (Yakovleva et al. 2016), and Ca (Belyaev et al. 2016; Barklem 2016b; Mitrushchenkov et al. 2017). Comparison with the available results of quantum calculations has shown that both model approaches provide reliable collision data, especially for processes with high and moderate rate coefficients, the processes which are the most important for non-LTE modeling.

Manganese is an element of significant astrophysical importance (Asplund 2005; Bergemann & Gehren 2007, 2008; Bergemann et al. 2013; Scott et al. 2015, see also references therein). In particular, manganese is of interest because it belongs to the iron-group elements. As noted by Jofré et al. (2015): “measuring accurate abundances of Mn is also important for studying the structure of our Galaxy”, and further “it is important for discussions of the formation history of the Galactic halo”. In addition, Hawkins et al. (2015) recently showed Mn to be one of the best candidates to distinguish Galactic components.

The iron-group elements have complicated electronic structures and, hence, potentials for interactions between hydrogen and the highly excited Mn-states considered here are not accessible by rigorous ab initio calculations. For this reason, the model asymptotic potential approach (Belyaev 2013a) is applied in the present work for MnH electronic structure calculations. This quantum model approach has been already applied to interactions of hydrogen with atoms and ions of some chemical elements: Al (Belyaev 2013b), Si (Belyaev et al. 2014b), Ca (Belyaev et al. 2016), Be (Yakovleva et al. 2016). It has been shown that the approach provides reliable potentials needed for nonadiabatic nuclear dynamical treatments. For the nonadiabatic nuclear dynamics, the model multichannel approach (see Belyaev 1993; Yakovleva et al. 2016, for details and references) has been chosen.

In the present study of manganese-hydrogen collisions, we take into account 21 low-lying covalent states and one (ground) ionic state. Transitions into other states in these collisions can be neglected². Cross sections and rate coefficients for partial inelastic processes (excitation, de-excitation, ion-pair formation and mutual neutralization) are calculated for all transitions between the states treated.

2. Model approach

The present study of inelastic low-energy manganese-hydrogen collisions continues a series of systematic treatments of inelastic

collisions of different atoms and positive ions with hydrogen atoms and its negative ions (Belyaev 2013b; Belyaev et al. 2014b, 2016; Yakovleva et al. 2016) by using the quantum model approaches within the framework of the Born-Oppenheimer formalism. Since these approaches have already been described in detail in previous papers, here we present only a brief description of the approach used.

The Born-Oppenheimer approach treats an inelastic collision process into two steps: (i) an electronic structure calculation of a considered (quasi-)molecule and (ii) a nonadiabatic nuclear dynamical study. In the present paper, the electronic structure calculation of the MnH molecule was performed by the asymptotic method (Belyaev 2013a), while the nonadiabatic nuclear dynamics was studied by means of the multichannel formulas (Belyaev 1993; Yakovleva et al. 2016) based on the Landau-Zener model.

It has been shown by the full quantum studies of collisions with hydrogen (Belyaev et al. 2010, 2012) that inelastic rate coefficients with large and moderate values are determined by long-range ionic-covalent interactions within molecular symmetries of the ground ionic molecular states. For this reason, the first step, the electronic structure calculation, was performed by a construction of the electronic Hamiltonian matrix in a diabatic representation as a function of the internuclear distance R . Within the asymptotic method, the Hamiltonian matrix for each ground-state ionic molecular symmetry is constructed from diagonal matrix elements for ionic and corresponding covalent molecular states and the off-diagonal matrix elements for ionic-covalent interactions (see Belyaev 2013a, for details). The diagonal terms should have correct asymptotic behavior. For single-electron transitions, the off-diagonal matrix elements, the exchange matrix elements, H_{jk} are obtained by means of the semi-empirical Olson-Smith-Bauer formula (Olson et al. 1971) $H_{jk}^{\text{OSB}}(R)$. However, some covalent molecular diabatic states are coupled with the ionic molecular diabatic states by two-electron transitions. In this case, the semi-empirical Olson-Smith-Bauer formula is not directly applicable, and Yakovleva et al. (2016) based on the results of (Belyaev 1993) have proposed estimating two-electron-transition exchange matrix elements H_{jk}^{2e} by the following expression:

$$H_{jk}^{2e}(R) = \left[H_{jk}^{\text{OSB}}(R) \right]^2 \times R. \quad (1)$$

The comparison with the accurate ab initio results for CaH (Mitrushchenkov et al. 2017) has shown that Eq. (1) provides reasonable estimates. Diagonalization of the electronic Hamiltonian matrix constructed by this way allows one to calculate the adiabatic potential energies for the MnH molecule, the data needed for the nuclear dynamics.

In the second step, the total inelastic transition probabilities for all transitions between considered states were calculated by means of the multichannel model. A nonadiabatic transition probability after a single traverse of a nonadiabatic region was calculated within the Landau-Zener model by the adiabatic-potential-based formula (see Belyaev & Lebedev 2011). Since the long-range nonadiabatic regions created by the ionic-covalent interaction are located in a particular order³, the analytic multichannel formulas (Belyaev & Tserkovnyi 1987; Belyaev 1993; Belyaev & Barklem 2003; Yakovleva et al. 2016) can be used for calculations of inelastic transition probabilities.

² Other states are higher-lying, create avoided crossings at large internuclear distances, larger than 100 atomic units, and, hence, have very small adiabatic splittings, which finally results in negligibly small inelastic transition probabilities, cross sections and rate coefficients, see, for example, (Belyaev et al. 2012).

³ This particular order means that the higher nonadiabatic region the larger internuclear distance of the region. This order is natural for avoided crossings created by the ionic-covalent interaction, see Fig. 1 below.

Two features that affect inelastic probabilities were taken into account in the present calculations. The first is a multi-passing of nonadiabatic regions for collision energies below the asymptote of the ionic channel, see (Devdariani & Zagrebin 1984; Belyaev 1985) for a three-channel case, as well as (Yakovleva et al. 2016) for a general case. This feature increases low-energy inelastic cross sections and finally low-temperature inelastic rate coefficients, which are the main interest for non-LTE modeling. The second feature is the tunneling effect, which takes place at large total angular momentum quantum numbers J . Taking this effect into account results in the additional factor for inelastic transition probabilities, see (Belyaev 1985), as well as (Yakovleva et al. 2016). Thus, the state-to-state inelastic probability $P_{if}(J, E)$ for a transition from an initial state i to a final state f for a given J and a given collision energy E can be calculated by using the multichannel formulas which are summarized by Yakovleva et al. (2016).

Cross sections and rate coefficients for exothermic ($k \rightarrow n$, $E_k > E_n$) and endothermic ($n \rightarrow k$) processes, $\sigma_{kn}(E)$, $K_{kn}(T)$ and $\sigma_{nk}(E)$, $K_{nk}(T)$, respectively, can be calculated by the following formulas:

$$\sigma_{kn}(E) = \frac{\pi \hbar^2 p_k^{\text{stat}}}{2\mu E} \sum_{J=0}^{\infty} P_{kn}(J, E) (2J+1), \quad (2)$$

$$\sigma_{nk}(E) = \sigma_{kn}(E - \Delta E_{kn}) \frac{p_n^{\text{stat}}}{p_k^{\text{stat}}} \frac{E - \Delta E_{kn}}{E}, \quad (3)$$

$$K_{kn}(T) = \sqrt{\frac{8}{\pi \mu (k_B T)^3}} \int_0^{\infty} E \sigma_{kn}(E) \exp\left(-\frac{E}{k_B T}\right) dE, \quad (4)$$

$$K_{nk}(T) = K_{kn}(T) \frac{p_n^{\text{stat}}}{p_k^{\text{stat}}} \exp\left(-\frac{\Delta E_{kn}}{k_B T}\right), \quad (5)$$

where $\Delta E_{kn} = E_k - E_n$ is the energy defect between the asymptotic energies of the channels k and n , T the temperature, p_j^{stat} the statistical probability for population of the channel j , k_B the Boltzmann constant, and μ the reduced nuclear mass. The rate coefficients for exothermic processes are usually weakly dependent on the temperature T , so it is better to compute them first for exothermic processes by means of Eq. (4), and then for endothermic ones by means of the detailed balance Eq. (5).

3. Manganese-hydrogen collisions

3.1. MnH electronic structure

The ground ionic $\text{Mn}^+(3d^5 4s^1 \ ^7S) + \text{H}^-(1s^2 \ ^1S)$ molecular state has the only symmetry: $^7\Sigma^+$, so inelastic transitions leading to high rate coefficients occur within this molecular symmetry. This restricts covalent molecular states effectively participating into the nonadiabatic nuclear dynamics, and finally this selects atomic states of Mn which should be taken into consideration. The 21 low-lying atomic states resulting in the $\text{MnH}(^7\Sigma^+)$ covalent molecular states, as well as the ground ionic $\text{Mn}^+ + \text{H}^-$ molecular state are listed in Table 1. These are the states taken into account in the present study. Higher-lying states are not efficiently coupled with these states and therefore not included into consideration.

We note that the considered covalent molecular states are mainly coupled with the ground ionic molecular state by single-electron transition exchange matrix elements, but three of the considered states, $\text{Mn}(3d^6(^5D)4p \ z \ ^6D^o)$, $\text{Mn}(3d^6(^5D)4p \ z \ ^6F^o)$, $\text{Mn}(3d^6(^5D)4p \ x \ ^6P^o) + \text{H}$, are coupled by two-electron transition ones. For this reason, as discussed above, the quantum

Fig. 1. $\text{MnH}(j \ ^7\Sigma^+)$ adiabatic potential energies obtained by the asymptotic method. The key for the labels j is collected in Table 1. The state labeled by $j = 22$ corresponds to the ionic $\text{Mn}^+ + \text{H}^-$ one, while other states are covalent.

model asymptotic approach was adjusted according to Eq. (1) (see also Yakovleva et al. 2016) for calculations of two-electron transition matrix elements.

The electronic structure adiabatic potentials were obtained by the asymptotic method as described above and are presented in Fig. 1. To the best of our knowledge, these potentials are calculated for the first time, except for the ground molecular state $\text{Mn}(3d^5 4s^2 \ ^6S) + \text{H}(1s^2 \ ^2S)$ (Blint et al. 1975), but a single potential does not allow one to consider a nonadiabatic nuclear dynamics.

The calculated adiabatic potentials depicted in Fig. 1 clearly show a series of the avoided-crossing regions, where nonadiabatic transitions take place. The computed long-range adiabatic potentials allowed us to calculate inelastic transition probabilities, cross sections and rate coefficients, as discussed above.

3.2. Cross sections and rate coefficients

Cross sections and rate coefficients were calculated by means of Eqs. (2)–(5) based on inelastic transition probabilities, which were in turn computed by the multichannel formulas. The partial inelastic cross sections of manganese-hydrogen collisions for the energy range 10^{-4} – 10^2 eV and the partial inelastic rate coefficients for the temperature range 1000–10 000 K were calculated for all transitions between the scattering states presented in Table 1.

It has been shown in our previous papers that the largest cross sections correspond to mutual neutralization processes and these processes play an important role in non-LTE modeling. It is also the case for manganese-hydrogen collisions. For this reason, Fig. 2 presents the energy dependence of the cross sections for the mutual neutralization processes: $\text{Mn}^+(3d^5 4s \ ^7S) + \text{H}^-(1s^2 \ ^1S) \rightarrow \text{Mn}^* + \text{H}$, that is, for the transitions $j = 22 \rightarrow k$ (the key for scattering channels is written in Table 1). It is seen that the scatter of the inelastic cross sections is up to several orders of magnitude. The largest cross sections correspond to the mutual neutralization processes into the final states $\text{Mn}(3d^5 4s(^7S)5s \ e \ ^6S)$, $\text{Mn}(3d^5 4s(^7S)5p \ y \ ^8P^o)$, $\text{Mn}(3d^5 4s(^7S)5s \ e \ ^8S)$, $\text{Mn}(3d^5 4s(^7S)4d \ e \ ^8D) + \text{H}(1s^2 \ ^2S)$, the states labeled by $k = 7, 11, 6, 12$, respectively. These cross sections, as well as those with the second largest values are

Table 1. MnH($j\ ^7\Sigma^+$) molecular states, the corresponding asymptotic atomic states (scattering channels), the manganese terms, the asymptotic energies ($\bar{J}$ -average experimental values taken from NIST; Kramida et al. 2012) with respect to the ground-state level, the electronic bound energies E_j , and the statistical probabilities for population of the molecular states.

j	Asymptotic atomic states	Mn terms	Asymptotic energies (eV)	Bound energies E_j (eV)	p_j^{stat}
1	Mn($3d^5 4s^2$) + H($1s\ ^2S$)	a 6S	0.0	-7.43404	0.5833
2	Mn($3d^6(^5D)4s$) + H($1s\ ^2S$)	a 6D	2.14508	-5.28896	0.1167
3	Mn($3d^5(^6S)4s4p\ ^3P^\circ$) + H($1s\ ^2S$)	z $^8P^\circ$	2.30260	-5.13144	0.1458
4	Mn($3d^5(^6S)4s4p\ ^3P^\circ$) + H($1s\ ^2S$)	z $^6P^\circ$	3.07387	-4.36017	0.1944
5	Mn($3d^5(^6S)4s4p\ ^1P^\circ$) + H($1s\ ^2S$)	y $^6P^\circ$	4.43088	-3.00315	0.1944
6	Mn($3d^5 4s(^7S)5s$) + H($1s\ ^2S$)	e 8S	4.88886	-2.54518	0.4375
7	Mn($3d^5 4s(^7S)5s$) + H($1s\ ^2S$)	e 6S	5.13343	-2.30061	0.5833
8	Mn($3d^6(^5D)4p$) + H($1s\ ^2S$)	z $^6D^\circ$	5.20176	-2.23228	0.1167
9	Mn($3d^6(^5D)4p$) + H($1s\ ^2S$)	z $^6F^\circ$	5.38961	-2.04443	0.0833
10	Mn($3d^6(^5D)4p$) + H($1s\ ^2S$)	x $^6P^\circ$	5.59255	-1.84149	0.1944
11	Mn($3d^5 4s(^7S)5p$) + H($1s\ ^2S$)	y $^8P^\circ$	5.70411	-1.72993	0.1458
12	Mn($3d^5 4s(^7S)4d$) + H($1s\ ^2S$)	e 8D	5.79126	-1.64278	0.0875
13	Mn($3d^5 4s(^7S)4d$) + H($1s\ ^2S$)	e 6D	5.85360	-1.58043	0.1167
14	Mn($3d^5 4s(^7S)5p$) + H($1s\ ^2S$)	w $^6P^\circ$	5.89743	-1.53661	0.1944
15	Mn($3d^5(^4P)4s4p\ ^3P^\circ$) + H($1s\ ^2S$)	y $^6D^\circ$	5.92037	-1.51367	0.1167
16	Mn($3d^5(^4P)4s4p\ ^3P^\circ$) + H($1s\ ^2S$)	y $^6F^\circ$	5.97253	-1.46151	0.0833
17	Mn($3d^5 4s(^5S)5s$) + H($1s\ ^2S$)	f 6S	6.12672	-1.30732	0.5833
18	Mn($3d^5(^4P)4s4p\ ^3P^\circ$) + H($1s\ ^2S$)	v $^6P^\circ$	6.19628	-1.23775	0.1944
19	Mn($3d^5 4s(^7S)6s$) + H($1s\ ^2S$)	f 8S	6.21875	-1.21529	0.4375
20	Mn($3d^5 4s(^7S)6s$) + H($1s\ ^2S$)	g 6S	6.31138	-1.12266	0.0833
21	Mn($3d^5(^4D)4s4p\ ^3P^\circ$) + H($1s\ ^2S$)	x $^6F^\circ$	6.32861	-1.10543	0.5833
22	Mn $^+(3d^5 4s\ ^7S)$ + H $^-(1s^2\ ^1S)$	–	6.68004	-0.754	1.0

Notes. The electronic bound energies are the same as the asymptotic energies, but measured from the ionization limit Mn $^+(3d^5 4s\ ^7S)$ + H($1s\ ^2S$); the differences between the asymptotic energy values and the bound energy values are equal to the ionization potential $I_{\text{Mn}} = 7.43404$ eV.

depicted in Fig. 3. The states with the largest and the second largest cross sections are located in the optimal window for the final electronic bound energies in accordance with the general role, see (Belyaev & Yakovleva 2017) and discussion below.

It is interesting to notice that the cross sections for transitions $j = 22 \rightarrow k = 1-7$ increase with collision energies above 1 eV while all the other neutralization cross sections decrease, see Figs. 2 and 3. This is connected with the shape of the relative potential energy curves, that is, the result of the fact that the potential energy splittings between low-lying states ($k = 1-7$) are rather large at the corresponding nonadiabatic regions (see Fig. 1), so the nonadiabatic transition probabilities and cross sections increase at relatively high collision energies, while for higher-lying avoided crossings ($k = 8-21$) the splittings are small leading to decrease of the corresponding transition probabilities and cross sections.

Rate coefficients $K_{if}(T)$ for the excitation, de-excitation, mutual neutralization and ion-pair formation processes in manganese-hydrogen collisions were calculated in the present work and published at the CDS for the temperature range $T = 1000-10\,000$ K. These rate coefficients for selected temperatures and for the processes from the optimal windows are presented in Table A.1. For the temperature $T = 6000$ K, the rate coefficients for the inelastic processes in manganese-hydrogen collisions are also shown in Fig. 4 in the form of graphical representation. It is seen that the highest rate coefficients correspond to the mutual neutralization processes. The rate coefficients $K_{if}(T = 6000\text{ K})$

Fig. 2. Manganese-hydrogen mutual neutralization cross sections for all inelastic channels. See Table 1 for the key of the channel labels.

for these processes ($i = 22 \equiv$ ionic) are depicted in Fig. 5 as a function of the electronic bound energy E_f for the final atomic state f (see Table 1 for the bound energies).

We can see that the highest rate coefficients correspond to the mutual neutralization processes with single-electron transitions from the optimal windows in the vicinity of the electronic bound energy $E_f = -2$ eV in accordance with the general

Fig. 3. Energy dependence of the cross sections for the mutual neutralization processes in $\text{Mn}^+ + \text{H}^-$ collisions with the largest values. For the label key see Table 1.

Fig. 4. Graphical representation of the rate coefficient matrix (in cm^3/s) for the partial processes of excitation, de-excitation, mutual neutralization and ion-pair formation in $\text{Mn} + \text{H}$ and $\text{Mn}^+ + \text{H}^-$ collisions at temperature $T = 6000$ K. The key is as for Fig. 1.

behavior (Belyaev & Yakovleva 2017). Outside of the optimal windows in both directions, increasing and decreasing the electronic bound energy, results in decreasing the rate coefficients, see Fig. 5. The processes characterized by two-electron transitions ($22 \rightarrow 8, 9, 10$ at present) have much lower rate coefficients, typically lower by a couple of orders of magnitude, even for the processes from the most optimal window, see Eq. (1). We note that presence of short-range nonadiabatic regions can markedly increase rate coefficients for two-electron transitions, but keeps the highest rates, as observed by Mitrushchenkov et al. (2017) for calcium-hydrogen collisions; treating short-range regions is outside of the scope of the present paper.

As mentioned in our previous papers, all partial processes can be divided into three groups according to the values of their rate coefficients: the groups with the higher (i), moderate (ii) and low (iii) rate coefficients. The first group with the largest values of rate coefficients, larger than $10^{-8} \text{ cm}^3/\text{s}$, consists of the mutual neutralization processes into the final states $\text{Mn}(3d^5 4s(7S)5s \text{ e } ^6S)$, $\text{Mn}(3d^5 4s(7S)5p \text{ y } ^8P^\circ)$, $\text{Mn}(3d^5 4s(7S)5s \text{ e } ^8S)$, $\text{Mn}(3d^5 4s(7S)4d \text{ e } ^8D)$, the processes

Fig. 5. Rate coefficients (at temperature $T = 6000$ K) for the mutual neutralization processes as a function of the electronic bound energy for the final atomic state. Filled circles represent the results for single-electron transitions, stars for two-electron transitions.

Fig. 6. Temperature dependence of the rate coefficients for the processes from the first group.

$22 \rightarrow 7, 11, 6, 12$, respectively. For temperature $T = 6000$ K, the rate coefficients of these processes have the values $4.38 \times 10^{-8} \text{ cm}^3/\text{s}$, $2.72 \times 10^{-8} \text{ cm}^3/\text{s}$, $1.98 \times 10^{-8} \text{ cm}^3/\text{s}$ and $1.59 \times 10^{-8} \text{ cm}^3/\text{s}$, respectively, see also Table A.1. These processes together with their inverse processes, the ion-pair formation, are expected to be the most important in astrophysical applications. Temperature dependence of these processes, direct and inverse, are presented in Fig. 6. As we can see, the mutual neutralization rate coefficients demonstrate weak temperature dependence, while those for the ion-pair formation processes depend rather strong on the temperature.

The second group consists of the processes with moderate rate coefficients, that is, with values in the range 10^{-10} – $10^{-8} \text{ cm}^3/\text{s}$. This group includes many excitation, de-excitation, mutual neutralization and ion-pair formation processes. At temperature $T = 6000$ K, the rate coefficients with the largest values in this group correspond to the inelastic transitions $22 \rightarrow 5$ ($K_{225} = 6.49 \times 10^{-9} \text{ cm}^3/\text{s}$), 13 ($9.38 \times 10^{-9} \text{ cm}^3/\text{s}$), 14 ($5.92 \times 10^{-9} \text{ cm}^3/\text{s}$), 15 ($4.57 \times 10^{-9} \text{ cm}^3/\text{s}$), 16 ($2.25 \times 10^{-9} \text{ cm}^3/\text{s}$); $6 \rightarrow 5$ ($1.99 \times 10^{-9} \text{ cm}^3/\text{s}$), $6 \rightarrow 7$ ($2.23 \times 10^{-9} \text{ cm}^3/\text{s}$); $7 \rightarrow 6$ ($4.78 \times 10^{-9} \text{ cm}^3/\text{s}$), as well as their

Fig. 7. Temperature dependence of the rate coefficients for the processes from the second group.

inverse processes and some other processes, see, for example, Table A.1. Temperature dependence of rate coefficients for these processes are presented in Fig. 7.

Finally, the third group consists of inelastic processes with low rate coefficients, typically lower than 10^{-10} cm³/s. This group includes excitation and de-excitation processes involving the ground state ($j = 1$), the four low-lying excited states ($j = 2-5$), the three states which correspond to two-electron transitions ($j = 8-10$), and the six high-lying states ($j = 16-21$) but the ionic one.

The processes from the first and the second groups are expected to be important in astrophysical non-LTE applications, while the processes with low rate coefficients, the processes from the third group, are likely to be unimportant. Moreover, the rate coefficients of the processes from the first two groups are expected to have higher accuracy than those from the third group.

4. Conclusion

The present study of low-energy inelastic manganese-hydrogen collisions was performed by means of the model approach derived earlier. The approach is based on the electronic structure calculation by means of the asymptotic method followed by the nonadiabatic nuclear dynamical treatment by means of the multichannel model approach. The cross sections for the energy range 10^{-4} – 10^2 eV and the rate coefficients for the temperature range 1000–10000 K for all transitions between 21 covalent and one ionic states are calculated. We show that the largest values of the cross sections and the rate coefficients correspond to the mutual neutralization processes into the final states $\text{Mn}(3d^5 4s^7 S) 5s \text{ } ^6S$, $\text{Mn}(3d^5 4s^7 S) 5p \text{ } ^8P^\circ$, $\text{Mn}(3d^5 4s^7 S) 5s \text{ } ^8S$, $\text{Mn}(3d^5 4s^7 S) 4d \text{ } ^8D$, the processes with the rate coefficients of the values 4.38×10^{-8} cm³/s, 2.72×10^{-8} cm³/s, 1.98×10^{-8} cm³/s and 1.59×10^{-8} cm³/s, respectively, at temperature $T = 6000$ K. There are also many other processes with the rate coefficient values between 10^{-10} and 10^{-8} cm³/s, the processes forming the second group of the processes with the moderate rate coefficients. These inelastic processes from these two groups are likely to be important in

non-LTE astrophysical applications. Other processes, including those with two-electron transitions, have low rate coefficients and are expected to be less important in astrophysical modeling. Nevertheless, the rate coefficients for these processes are also estimated though with lower accuracy, while the accuracy of the rate coefficients with large and moderate values is quite high.

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Appendix A: Additional table

Table A.1. Rate coefficients $K_{if}(T)$ (in units of cm^3/s) at temperatures $T = 1000, 4000, 6000$, and $10\,000$ K for the processes from the optimal windows.

$T = 1000$ K													
i	f												
	5	6	7	8	9	10	11	12	13	14	15	16	22
5	–	3.56E-12	3.86E-14	2.12E-16	2.85E-16	8.05E-17	4.62E-17	1.08E-17	3.74E-18	1.78E-18	1.21E-18	5.88E-19	8.58E-21
6	1.63E-09	–	1.55E-10	8.06E-13	8.77E-13	2.06E-13	9.41E-14	2.09E-14	7.06E-15	3.31E-15	2.24E-15	1.09E-15	1.37E-17
7	4.02E-10	3.54E-09	–	1.56E-10	1.07E-10	1.85E-11	6.52E-12	1.37E-12	4.48E-13	2.08E-13	1.39E-13	6.75E-14	7.63E-16
8	9.78E-13	8.11E-12	6.88E-11	–	8.22E-13	6.60E-14	1.51E-14	2.92E-15	9.35E-16	4.30E-16	2.85E-16	1.42E-16	1.76E-18
9	8.28E-12	5.58E-11	2.98E-10	5.19E-12	–	1.24E-13	2.33E-14	4.33E-15	1.36E-15	6.21E-16	4.10E-16	2.06E-16	2.84E-18
10	5.76E-11	3.22E-10	1.27E-09	1.02E-11	3.04E-12	–	1.04E-13	1.72E-14	5.14E-15	2.27E-15	1.48E-15	7.17E-16	1.02E-17
11	9.06E-11	4.03E-10	1.23E-09	6.41E-12	1.57E-12	2.86E-13	–	1.93E-10	5.24E-11	2.24E-11	1.44E-11	6.82E-12	9.39E-14
12	3.50E-11	1.48E-10	4.24E-10	2.05E-12	4.81E-13	7.76E-14	3.19E-10	–	6.43E-11	2.44E-11	1.50E-11	6.74E-12	9.01E-14
13	3.32E-11	1.37E-10	3.82E-10	1.80E-12	4.15E-13	6.39E-14	2.38E-10	1.77E-10	–	5.28E-11	2.90E-11	1.18E-11	1.45E-13
14	4.37E-11	1.78E-10	4.90E-10	2.30E-12	5.26E-13	7.81E-14	2.82E-10	1.86E-10	1.46E-10	–	7.86E-11	2.36E-11	2.55E-13
15	2.33E-11	9.43E-11	2.57E-10	1.19E-12	2.71E-13	3.98E-14	1.41E-10	8.92E-11	6.29E-11	6.15E-11	–	1.65E-11	1.54E-13
16	1.48E-11	5.99E-11	1.63E-10	7.76E-13	1.78E-13	2.53E-14	8.78E-11	5.26E-11	3.34E-11	2.42E-11	2.16E-11	–	9.81E-14
22	9.55E-09	3.32E-08	8.14E-08	4.25E-10	1.09E-10	1.58E-11	5.34E-08	3.10E-08	1.82E-08	1.15E-08	8.87E-09	4.33E-09	–
$T = 4000$ K													
i	f												
	5	6	7	8	9	10	11	12	13	14	15	16	22
5	–	2.07E-10	2.96E-11	8.22E-14	3.15E-13	4.72E-13	1.96E-12	8.56E-13	4.33E-13	2.58E-13	1.95E-13	1.12E-13	1.87E-12
6	1.76E-09	–	1.60E-09	5.52E-12	2.06E-11	2.61E-11	7.53E-11	3.18E-11	1.59E-11	9.41E-12	7.09E-12	4.13E-12	5.11E-11
7	6.82E-10	4.34E-09	–	1.23E-10	3.44E-10	3.30E-10	6.51E-10	2.63E-10	1.29E-10	7.61E-11	5.68E-11	3.36E-11	3.18E-10
8	4.61E-13	3.65E-12	3.00E-11	–	2.39E-12	1.09E-12	1.16E-12	4.31E-13	2.07E-13	1.21E-13	9.01E-14	5.34E-14	3.72E-13
9	2.18E-12	1.67E-11	1.03E-10	2.95E-12	–	3.87E-13	3.55E-13	1.28E-13	6.12E-14	3.56E-14	2.63E-14	1.63E-14	1.19E-13
10	1.37E-11	8.93E-11	4.17E-10	5.63E-12	1.63E-12	–	2.48E-13	8.24E-14	3.92E-14	2.17E-14	1.59E-14	9.42E-15	7.47E-14
11	5.90E-11	2.67E-10	8.52E-10	6.23E-12	1.55E-12	2.57E-13	–	3.23E-10	1.40E-10	7.87E-11	5.65E-11	3.36E-11	2.65E-10
12	1.99E-11	8.72E-11	2.66E-10	1.79E-12	4.32E-13	6.60E-14	2.49E-10	–	7.81E-11	4.02E-11	2.79E-11	1.61E-11	1.19E-10
13	1.61E-11	6.95E-11	2.08E-10	1.37E-12	3.29E-13	5.01E-14	1.73E-10	1.25E-10	–	4.92E-11	3.14E-11	1.68E-11	1.12E-10
14	1.81E-11	7.80E-11	2.33E-10	1.52E-12	3.63E-13	5.26E-14	1.84E-10	1.21E-10	9.31E-11	–	5.41E-11	2.36E-11	1.34E-10
15	8.81E-12	3.77E-11	1.11E-10	7.25E-13	1.72E-13	2.47E-14	8.46E-11	5.41E-11	3.81E-11	3.47E-11	–	1.36E-11	6.65E-11
16	4.20E-12	1.82E-11	5.47E-11	3.57E-13	8.84E-14	1.22E-14	4.18E-11	2.59E-11	1.69E-11	1.26E-11	1.13E-11	–	2.72E-11
22	6.57E-09	2.11E-08	4.85E-08	2.33E-10	6.02E-11	9.01E-12	3.08E-08	1.79E-08	1.06E-08	6.69E-09	5.17E-09	2.54E-09	–
$T = 6000$ K													
i	f												
	5	6	7	8	9	10	11	12	13	14	15	16	22
5	–	3.65E-10	7.39E-11	1.47E-13	4.91E-13	8.69E-13	5.82E-12	2.64E-12	1.35E-12	8.07E-13	6.09E-13	3.38E-13	1.63E-11
6	1.99E-09	–	2.23E-09	5.78E-12	2.10E-11	3.17E-11	1.38E-10	6.12E-11	3.11E-11	1.85E-11	1.39E-11	7.91E-12	2.71E-10
7	8.62E-10	4.78E-09	–	9.57E-11	2.86E-10	3.27E-10	9.25E-10	3.93E-10	1.97E-10	1.17E-10	8.76E-11	5.06E-11	1.28E-09
8	3.91E-13	2.82E-12	2.18E-11	–	2.04E-12	1.11E-12	1.58E-12	6.20E-13	3.04E-13	1.80E-13	1.34E-13	7.77E-14	1.34E-12
9	1.34E-12	1.06E-11	6.71E-11	2.10E-12	–	3.29E-13	4.11E-13	1.57E-13	7.66E-14	4.48E-14	3.31E-14	2.01E-14	3.58E-13
10	8.22E-12	5.49E-11	2.65E-10	3.93E-12	1.14E-12	–	2.36E-13	8.34E-14	4.07E-14	2.26E-14	1.66E-14	9.58E-15	1.87E-13
11	5.12E-11	2.23E-10	6.97E-10	5.23E-12	1.32E-12	2.19E-13	–	2.90E-10	1.30E-10	7.34E-11	5.28E-11	3.07E-11	6.01E-10
12	1.65E-11	7.01E-11	2.11E-10	1.45E-12	3.59E-13	5.51E-14	2.06E-10	–	6.63E-11	3.46E-11	2.41E-11	1.36E-11	2.49E-10
13	1.27E-11	5.35E-11	1.59E-10	1.07E-12	2.63E-13	4.04E-14	1.38E-10	9.97E-11	–	3.99E-11	2.58E-11	1.35E-11	2.21E-10
14	1.38E-11	5.78E-11	1.71E-10	1.15E-12	2.79E-13	4.08E-14	1.42E-10	9.44E-11	7.24E-11	–	4.23E-11	1.83E-11	2.53E-10
15	6.51E-12	2.73E-11	8.02E-11	5.37E-13	1.29E-13	1.88E-14	6.42E-11	4.13E-11	2.93E-11	2.65E-11	–	1.03E-11	1.23E-10
16	2.86E-12	1.23E-11	3.66E-11	2.46E-13	6.20E-14	8.56E-15	2.95E-11	1.84E-11	1.21E-11	9.09E-12	8.17E-12	–	4.78E-11
22	6.49E-09	1.98E-08	4.38E-08	2.01E-10	5.22E-11	7.90E-12	2.72E-08	1.59E-08	9.38E-09	5.92E-09	4.57E-09	2.25E-09	–
$T = 10\,000$ K													
i	f												
	5	6	7	8	9	10	11	12	13	14	15	16	22
5	–	6.29E-10	1.68E-10	2.31E-13	5.45E-13	1.08E-12	1.32E-11	6.04E-12	3.09E-12	1.82E-12	1.36E-12	7.12E-13	9.91E-11
6	2.41E-09	–	2.98E-09	5.36E-12	1.65E-11	2.81E-11	2.02E-10	9.10E-11	4.64E-11	2.74E-11	2.05E-11	1.11E-11	1.06E-09
7	1.14E-09	5.28E-09	–	6.46E-11	1.90E-10	2.48E-10	1.06E-09	4.63E-10	2.34E-10	1.38E-10	1.03E-10	5.72E-11	3.89E-09
8	3.40E-13	2.05E-12	1.40E-11	–	1.39E-12	8.60E-13	1.68E-12	6.82E-13	3.38E-13	1.99E-13	1.48E-13	8.34E-14	3.56E-12
9	7.10E-13	5.62E-12	3.65E-11	1.23E-12	–	2.21E-13	3.85E-13	1.53E-13	7.53E-14	4.39E-14	3.23E-14	1.89E-14	8.27E-13
10	4.14E-12	2.83E-11	1.41E-10	2.26E-12	6.54E-13	–	1.91E-13	7.07E-14	3.47E-14	1.93E-14	1.41E-14	7.80E-15	3.76E-13
11	4.33E-11	1.73E-10	5.12E-10	3.76E-12	9.70E-13	1.63E-13	–	2.24E-10	1.02E-10	5.74E-11	4.12E-11	2.30E-11	1.12E-09
12	1.32E-11	5.19E-11	1.49E-10	1.01E-12	2.56E-13	4.00E-14	1.49E-10	–	4.85E-11	2.54E-11	1.77E-11	9.59E-12	4.34E-10
13	9.67E-12	3.79E-11	1.08E-10	7.20E-13	1.81E-13	2.82E-14	9.66E-11	6.96E-11	–	2.79E-11	1.81E-11	9.14E-12	3.68E-10
14	9.99E-12	3.93E-11	1.12E-10	7.44E-13	1.85E-13	2.74E-14	9.58E-11	6.38E-11	4.89E-11	–	2.85E-11	1.21E-11	4.08E-10
15	4.59E-12	1.81E-11	5.13E-11	3.41E-13	8.37E-14	1.24E-14	4.24E-11	2.75E-11	1.96E-11	1.75E-11	–	6.69E-12	1.94E-10
16	1.83E-12	7.43E-12	2.16E-11	1.46E-13	3.71E-14	5.20E-15	1.79E-11	1.13E-11	7.49E-12	5.65E-12	5.08E-12	–	7.26E-11
22	6.93E-09	1.93E-08	4.01E-08	1.70E-10	4.44E-11	6.84E-12	2.39E-08	1.39E-08	8.24E-09	5.20E-09	4.01E-09	1.98E-09	–

Notes. The rate coefficients with small values are not included in this table, except for the processes corresponding to two-electron transitions (the states $i, f = 8-10$).