Processes of $H - H^+ - e$ and $H_2^+ - e$ recombination in the weakly-ionized layers of the solar atmosphere

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Abstract. The influence of the $H-H^+-e$ and H_2^+-e chemi - recombination processes on the highly excited hydrogen atom population in the photosphere and lower part of the chromosphere has been considered. It has been shown that these chemi - recombination processes have an important role in the large region around the temperature minimum in the Solar atmosphere, where they are comparable to the other relevant recombination processes, or even dominant and that they should be taken into account for the modelling of the weakly ionized layers in the Solar atmosphere.

Key words: molecular data - Sun: atmosphere

1. Introduction

In several previous papers (Mihajlov & Ljepojević, 1982 and Mihajlov et al. 1992, 1996), chemi-recombination processes during the free electron scattering on the quasi-molecular collisional complexes $H(1s) + H^+$ and molecular ions H_2^+ in the weakly bound rhovibrational states, have been introduced and investigated. It was assumed that these molecular ions are in the ground electronic state $X^2\Sigma_g^+(1s\sigma_g)$. The mentioned chemi-recombination processes are

$$H_2^+ + e \Rightarrow H^*(n) + H(1s),$$
 (1a)

$$H(1s) + H^+ + e \Rightarrow H^*(n) + H(1s),$$
 (1b)

where $H^*(n)$ denotes hydrogen atom in a highly excited (Rydberg) state with the principal quantum number $n \leq 4$. It has been shown that in partially ionized plasma the processes (1a) and (1b) may be significant for the $H^*(n)$ atom populations. This conclusion has been derived from the comparison of the (1a,b) processes with the electron - electron - ion recombination processes whose importance for hydrogen plasmas is well known (see e.g. Bates et al. 1962ab).

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In this paper we will consider the (1a,b) processes from the aspect of their influence on $H^*(n)$ atom populations of solar photosphere and lower part of chromosphere. We point out here that the taking into account of these processes may be particularly important when the conditions of LTE, concerning the excited atom population distribution function, are not satisfied. Such situation exist just for the above mentioned parts of the solar atmosphere (due to their small optical depth), which has been pointed out in Maltby et al. (1986) and Vernazza et al. (1981). The principal aim of this paper is to show that for particular layers of the solar atmosphere, the chemi - recombination processes (1a,b) could be comparable or sometimes even more important that the processes of the electron - electron ion recombination as well as with the processes of electron ion photorecombination, which have a particularly important role in the solar atmosphere. Consequently, we will show that the (1a,b) processes must be taken into account when modelling the solar atmosphere, together with other relevant recombination processes.

2. Theory

In accordance with Mihajlov & Ljepojević, 1982 and Mihajlov et al. 1992, 1996, recombination processes (1a,b) will be treated as the result of the energy exchange within the electronic component of the $H_2^+ + e$ or $H + H^+ + e$ system, which is caused by dipole interaction of the electron e with the ion atomic subsystem H_2^+ or $H + H^+$. Here we have in mind that the energy exchange is connected with the transition of the just mentioned ion - atomic subsystems from the orbital $1s\sigma_q$ to the first excited orbital $2p\sigma_u$ and the simultaneous transition of the electron e from the free state to the highly excited bound state. It is assumed that the transition $1s\sigma_q \rightarrow 2p\sigma_u$ is performed without the energy exchange between electron and cores (protons). Also, it is assumed that the change of the electronic state of the $H_2^+ + e$ or $H + H^+ + e$ system, during the scattering of the free electron on the molecular ion or the quasi - molecular collisional complex, can happen only once. The difference between the (1a) and (1b) processes is that the ion - atomic subsystem H_2^+ is in the initial electronic state $X^2\Sigma_q^+(1s\sigma_q)$ with the proba-

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bility equal to 1, and the subsystem $H + H^+$ with the probability equal to 1/2. Consequently, the processes (1a) and (1b) may be treated as the corresponding channels of a more general chemirecombination process (1) which is similar to the process of the direct disociative recombination.

Concerning the nuclei motion, it is treated classically for the (1b) processes where the ion - atomic subsystem is in the state of free motion, as well as for the (1a) processes, where within the input channel the ion - atomic subsystem is in a bound state. Here we take into account the assumption that these bound states are near the dissociation threshold, where the mentioned classical treatment is valid.

We will consider here the total influence of the (1a,b) chemirecombination processes on the $H^*(n)$ atom populations in the considered Solar plasma. Consequently, as a quantitative characteristic of the above mentioned influence we will use the total chemi - recombination fluxes $I_r^{(ab)}(n) = I_r^{(a)}(n) + I_r^{(b)}(n)$, where $I_r^{(a)}(n)$ and $I_r^{(b)}(n)$ are the partial fluxes corresponding to the (1a) and (1b) chemi - recombination processes, respectively. It should be pointed out that the partial fluxes are denoted here as in our previous papers (Mihajlov et al. 1992, 1996). In Mihailov et al. (1992, 1996) the recombination processes (1a,b) were treated for the more general non-equillibrium case for $T_e > T_a$, where T_e and T_a are the temperatures characterizing electronand ion/atom - component. Here however, we take into account that in the standard models of solar photosphere (Maltby et al. 1986) and chromosphere (Vernazza et al. 1981), it has been taken that $T_a = T_e = T$. Consequently, we will assume that $I_r^{(a,b,ab)}(n) = I_r^{(a,b,ab)}(n;T).$

According to Mihajlov et al. (1992, 1996), we will treat both partial chemi - recombination fluxes (for the case $T_a = T_e = T$) in the same form, i.e. as $I_r^{(a,b)}(n) = K_r^{(a,b)}(n;T)N(e)N(H^+)N(1)$, where N(e) and $N(H^+)$ are the electron and proton densities and N(1) is the density of H(1s) atoms. Here $K_r^{(a)}(n;T)$ replaces the quantity $K_{dr}^{(a)}(n;T)N(H_2^+)[N(H^+)N(1)]^{-1}$, where $N(H_2^+)$ is the $H_2^+(1s\sigma)$ molecular ion density, and the $K_{dr}^{(a)}$ is the usuall disociative recombination rate coefficient. This enables the total chemi-recombination flux $I_r^{(ab)}(n)$ to be presented in the form:

$$I_r^{(ab)}(n;T) = K_r^{(ab)}(n;T)N(e)N(H^+)N(1), \tag{2}$$

where $K_r^{(ab)}(n;T)=K_r^{(a)}(n;T)+K_r^{(b)}(n;T)$. The advantage of such expression for the total chemi - recombination rate coefficient $K_r^{(ab)}(n;T)$ is, since the H_2^+ molecular ion density is absent in Eq. (2). This approach is constructive when the block of the weakly - bound rhovibrational states of the $H_2^+(1s\sigma)$ molecular ion, essential for the (1a) processes, is in the dissociative - associative equilibrium with the H(1s) and H^+ components (with the same temperature T). Here, the assumption on existance of such dissociative - associative equilibrium is adopted on the basis of the above mentioned models of the solar atmosphere (Maltby et al. 1986, Vernazza et al. 1981). Namely, in these models the existance of LTE is assumed, when the radiation transfer out of the solar atmosphere is not taken into account. If such transfer is taken into account, some deviations from LTE

are considered (in these models) which are not important for the discussed dissociative - associative equilibrium.

We will use here the total rate coefficient $K_r^{(ab)}(n;T)$ as in Mihajlov et al. (1996), i.e. as

$$K_r^{(ab)}(n;T) = \frac{(2\pi)^{5/2}}{3\sqrt{3}} \frac{(\hbar e a_0)^2}{(mkT)^{3/2}}$$

$$\frac{\exp(I_n/kT)}{n^3} \int_0^{R_n} \exp\left[-\frac{U_2(R)}{kT}\right] \frac{R^4 dR}{a_2^5}, \tag{3}$$

where the upper integration limit R_n is the root of the equation

$$U_2(R) - U_1(R) = I_n. (4)$$

Here, $I_n = R_y/n^2$ is the ionization potential of the $H^*(n)$ atom, while $U_1(R)$ and $U_2(R)$ are the adiabatic terms of the ground $(1\Sigma_g)$ and the first excited $(1\Sigma_u)$ electronic state of the molecular ion H_2^+ , whose values are taken from Bates et al (1953).

According to the same paper, the lower integration limit instead of zero is taken as a_0 in Eq. (3) for the concrete calculations. The values of the R_n , for n=4-10, are given in Mihajlov et al (1996) and here we will treat the processes (1a,b) just within this range of values for n.

The processes (1a,b) with n = 2, 3 are not treated here since our considerations are based on the previous papers (Mihajlov et al., 1992; Mihajlov et al., 1996), where only the region $n \ge 4$ was treated. This was imposed by the conditions of applicability of the used theory. For example, for n = 3 already the change of the electronic state of the $H_2^+ + e$ or $H + H^+ + e$ system (during the scattering of the free electron on the molecular ion or the quasi - molecular collisional complex) can happen more than once. Consequently, each of the processes (1a) and (1b) obtains the multi - channel character. That is why the inclusion of the processes (1a) and (1b) imposes a different approach. One of the possible solutions could be the adequate version of MQDT method, which was firstly developed for atoms (M. J. Seaton, 1966; see also U. Fano, 1970). In the case of a molecular system such methods have also been developing for a long time, and for the processes of dissociative recombination of the (1a) type some preliminary results already exist (see Giusti-Suzor, 1989; Hickman, 1989; and references therein).

The behaviour of the total rate coefficient $K_r^{(ab)}(n;T)$ as a function of the temperature T for n=4-10, is shown in Table 1. This table covers the 4000 K $\leq T \leq$ 6500 K range, which is of interest for further consideration.

3. Results and discussions

The (1b) chemi - recombination processes may be significant only when the neutral atom component is dominant. Consequently, we will consider that part of the Solar atmosphere where the ionization degree is small enough. We will use here the Solar atmosphere plasma parameter data presented in Vernazza et al. (1981), similarly to Mihajlov et al. (1993, 1994), where the radiation processes during $H^+ + H(1s)$ collisions were considered.

Table 1. The values of the chemi-recombination rate coefficient $K_r^{(ab)}(n;T)$ in the case of the $T_a=T_e=T$, where T_a and T_e denote the temperatures of the atom/ion end electron components respectively, and n is the principal quantum number.

	$10^{28} K_r^{(ab)}(n;T) / [cm^6 s^{-1}]$									
T/[K]	n=4	n=5	n=6	n=7	n=8	n=9	n=10			
4000	2.7824	1.6622	1.1602	.8884	.7201	.6038	.5203			
4250	2.4277	1.4864	1.0512	.8105	.6593	.5537	.4774			
4500	2.1421	1.3403	.9588	.7438	.6069	.5104	.4402			
4750	1.9083	1.2172	.8796	.6860	.5612	.4726	.4077			
5000	1.7143	1.1123	.8111	.6356	.5213	.4394	.3792			
5250	1.5512	1.0221	.7514	.5907	.4859	.4100	.3539			
5500	1.4126	.9438	.6988	.5515	.4546	.3839	.3314			
5750	1.2938	.8752	.6524	.5166	.4265	.3604	.3112			
6000	1.1909	.8148	.6110	.4854	.4013	.3394	.2930			
6250	1.1011	.7613	.5739	.4572	.3786	.3203	.2766			
6500	1.0223	.7135	.5406	.4318	.3580	.3030	.2617			

Here we will use the chromospheric model C of Vernazza et al. (1981), since in this article temperatures, electron and ion densities are given, as well as the $H^*(n)$ atom densities as a function of the height h. The atomic densities calculations where performed there within the $1 \le n \le 8$ range. These atom densities are denoted here as N(n).

We consider here the height range -75km $\leq h \leq$ 1605km with the plasma conditions illustrated in Table 2. In this table, first of all, temperatures T and N(e)/N(H) ratios (where the N(H) is the total hydrogen density) from Vernazza et al. (1981) are given. One can see that the temperature changes from 4170 K up to 6440 K for the presented h values i.e. within the temperature range presented in Table 1. The N(e)/N(H) ratio characterizes the plasma ionization degree, as long as its value remains much smaller than one. Table 2 shows that the N(e)/N(H) ratio values remain smaller than 0.1 within the whole considered range and that for -75km $\leq h <$ 1180km these values decrease below 0.01. Also, Table 2 shows the values of

$$\eta(n) = \frac{N(n)}{N_{eq}(n)},\tag{5}$$

as a function of h. Here, the $N_{eq}(n)$ denotes the equilibrium density of the $H^*(n)$ atoms which was determined by us, with the T, N(e) and $N(H^+)$ taken from Vernazza et al. (1981) corresponding to the given h. From Table 2 one can see that the $\eta(n)$ parameter values vary between 0.6 and 1.2, which implies the difference of the N(n) values from the equilibrium ones. These differences confirm that the chemi - recombination processes (1a,b), not taken into account in Vernazza et al. (1981) for N(n) calculations, may be significant in comparison with the other recombination processes within the h range considered.

In order to estimate the importance of the (1a,b) chemirecombination processes, we will compare them at first with the photorecombination processes

$$H^+ + e \Rightarrow H^*(n) + h\omega, \tag{6}$$

Table 2. Basic plasma parameters, for the solar chromospheric model of Vernazza et. al. (1981, model C), as a function of height h. The parameter $\eta(n) = N(H^*)(n)/N_{eq}(H^*)(n)$, where $N_{eq}(H^*)(n)$ is the equilibrium density of $H^*(n)$ atoms which corresponds to the electron density N(e) and the proton density $N(H^*)$ from the same model.

			$\eta(n)$						
h/[km]	T/[K]	N(e)/N(H)	n=4	n=5	n=6	n=7	n=8		
1605	6440	.9403E-01	.9860	.9381	.9316	.9014	.8996		
1515	6370	.6160E-01	1.1407	1.0670	1.0503	1.0119	1.0088		
1380	6280	.3344E-01	1.1496	1.0492	1.0248	.9848	.9820		
1280	6220	.1782E-01	1.1271	1.0138	.9869	.9473	.9445		
1180	6150	.1031E-01	1.1946	1.0618	1.0269	.9830	.9798		
1065	6040	.5464E-02	1.2192	1.0721	1.0326	.9871	.9891		
980	5925	.3308E-02	1.2286	1.0762	1.0348	.9882	.9853		
905	5755	.1891E-02	1.1996	1.0563	1.0170	.9710	.9683		
855	5650	.1308E-02	1.1747	1.0392	1.0015	.9560	.9537		
755	5280	.4741E-03	1.0444	.9547	.9302	.8899	.8889		
705	5030	.2611E-03	.9362	.8795	.8668	.8318	.8321		
655	4730	.1686E-03	.8011	.7878	.8549	.7641	.7659		
605	4420	.1370E-03	.6752	.7004	.7205	.6981	.7015		
555	4230	.1254E-03	.6190	.6661	.6936	.6720	.6755		
515	4170	.1190E-03	.6195	.6745	.7031	.6795	.6828		
450	4220	.1132E-03	.6884	.7405	.7646	.7357	.7380		
350	4465	.1112E-03	.8518	.8812	.8937	.8564	.8572		
250	4780	.1155E-03	.9771	.9862	.9898	.9479	.9478		
150	5180	.1317E-03	1.0323	1.0397	1.0397	.9973	.9967		
100	5455	.1553E-03	1.0290	1.0438	1.0444	1.0042	1.0035		
50	5840	.2306E-03	1.0273	1.0260	1.0416	1.0040	1.0035		
0	6420	.5517E-03	1.0191	1.0359	1.0366	1.0029	1.0024		
-25	6910	.1227E-02	1.0167		1.0335	1.0022	1.0016		
-50	7610	.3527E-02	1.0161	1.0303	1.0309	1.0024	1.0021		
-75	8320	.8821E-02	1.0154	1.0285	1.0291	1.0031	1.0027		

for the $n \ge 4$ range. As a quantitative characteristic of the relative influence of the (1a,b) chemi - recombination processes and the photorecombination processes (6) we will use the quantity

$$F_{phr}^{(ab)}(4;8) = \frac{\sum_{4}^{8} I_{r}^{(ab)}(n;T)}{\sum_{4}^{8} I_{phr}(n;T)},$$
 (7)

where $I_{phr}(n;T)$ denotes the photorecombination flux conditioning the process (6) for given n. In order to determine the $F_{phr}^{(ab)}(4;8)$ values, Eqs (2-4) have been used for $\Sigma_4^8 I_r^{(ab)}(n;T)$ calculations, while $\Sigma_4^8 I_{phr}(n;T)$ is estimated on the basis of data from Vernazza et al. (1981). Fig. 1 illustrates the behavior of the $F_{phr}^{(ab)}(4;8)$ quantity for 350 km $\leq h \leq$ 905 km. We show only this height range, since for h > 905 km the values of quantity $F_{phr}^{(ab)}(4; 8)$ decrease below 0.01, while for h < 350 km these values continue to increase monotonically. One can see in Fig. 1 that above around 700 km the influence of the (1a,b) processes is much smaller in comparison with the photorecombination processes ($F_{phr}^{(ab)}(4; 8) < 0.1$). For 650 km < h < 700km the influence of both processes is comparable and for h <650 km the (1a,b) chemi - recombination processes are dominant in comparison with the photorecombination processes (6) for $n \geq 4$.

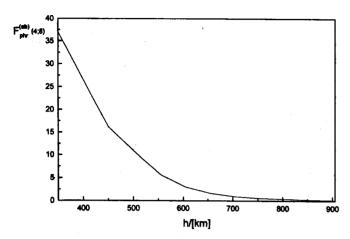


Fig. 1. The behaviour of the quantity $F_{phr}^{(ab)}(4;8)$, given by Eq. (7), as a function of height h.

This conclusion is not connected with our choice of the n=8 as the upper limit of the considered n values region. Namely, our estimates performed in order to check this conclusion show that if we change even only $\Sigma_4^8 I_{phr}(n;T)$ with the sum for all $n\geq 4$, which have sense for given T and N(e), the ratio values on Eq. (6) right side will be changed around 20 percent. It is clear that this change will be even smaller if $\Sigma_4^8 I_r^{(ab)}(n;T)$ in Eq. (7) will be changed in the adequate way. The performed estimates are possible with the help of results of the photorecombination fluxes calculations in Oesterbrock (1974) analyzed in Vernazza et al. (1981).

In the next step we will compare the (1a,b) chemirecombination processes with the electron - electron - ion recombination processes

$$H^+ + e + e \Rightarrow H^*(n) + e, \tag{8}$$

for the same $n \ge 4$ range. As a quantitative characteristic of the relative influence of the (1a,b) chemi - recombination processes and the electron - electron - ion recombination processes (8) we will first of all use the quantity

$$F_{eei}^{(ab)}(4;8) = \frac{\sum_{4}^{8} I_{r}^{(ab)}(n;T)}{\sum_{5}^{8} I_{e}^{eei}(n;T)},$$
(9)

where $I_r^{eei}(n;T)$ denotes the electron - electron - ion recombination flux conditioning the process (8) for given n, taken here in the form

$$I_r^{eei}(n) = \alpha_r^{eei}(T)[N(e)]^2 N(H^+).$$
 (10)

For determination of the $F_{eei}^{(ab)}(4;8)$ values, the $\alpha_r^{eei}(T)$ rate coefficients have been calculated here by using the corresponding expressions in Vriens et al. (1980). The behavior of the $F_{eei}^{(ab)}(4;8)$ quantity for $0 \text{ km} \leq h \leq 1065 \text{ km}$ illustrates Fig. 2. This Fig. shows that around 450 km, the (1a,b) chemi-recombination processes become even more influent than the electron-electron-ion recombination processes (8), while within $0 \text{ km} \leq h \leq 750 \text{ km}$ range both processes are comparable

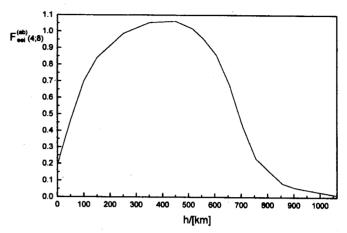


Fig. 2. The behaviour of the quantity $F_{eei}^{(ab)}(4;8)$, given by Eq. (9), as a function of height h.

 $(F_{eei}^{(ab)}(4;8) > 0.2)$. For h < 0km and h > 750km, the influence of the chemi - recombination processes becomes small in comparison with electron - electron - ion recombination processes $(F_{eei}^{(ab)}(4;8) < 0.1 \text{ for } h < -25$ km and h > 850km).

Besides the $F_{eei}^{(ab)}(4;8)$ quantity, we will introduce also the quantities $f_{eei}^{(ab)}(n) = I_r^{(ab)}(n,T)/I_r^{eei}(n,T)$, characterizing the relative influence of the (1a,b) chemi - recombination processes in comparison with the electron - electron - ion recombination processes (8), on the $H^*(n)$ atom populations for the given n. From Eq. (2) and (10) we have that

$$f_{eei}^{(ab)}(n) = \frac{K_r^{(ab)}(n, T)}{\alpha_r^{eei}(T)} \frac{N(1)}{N(e)}.$$
 (11)

N(1)/N(e)ratio may be with $[N(e)/N(H)]^{-1}$ from Table 2, for the $h \le 750$ km range, practically without the decrease of accuraccy. The behavior of the $f_{eei}^{(ab)}(n)$ quantities as a function of height h for n = 4 - 8is shown in Fig. 3. One can see in Fig. 3 that for n values considered, the chemi - recombination processes are comparable with the electron - electron - ion recombination processes (for n = 6 - 8) or dominant (for n = 4, 5) within a wide h range which lower limit changes for different n from -75 km up to 50 km and the upper one from 650 km up to 750km. For n = 4and 5 the h range where the relative influence of the chemirecombination processes remains comparable, is up to around 1200km.

The specific significance of the $f_{eei}^{(ab)}(n)$ quantities is in the fact that they are in the same time ratios of the total fluxes $I_{tot}^{(ab)}(n;T)$ and $I_{tot}^{eei}(n;T)$ characterizing the influence of the ionization processes inverse to the (1a,b) and the (8) recombination process. Namely, in the partially ionized plasma, the (1a,b) chemi - recombination processes occure together with the inverse chemi - ionization processes due to $H^*(n) + H(1s)$ collisions, while the electron - electron - ion processes (8) occure together with the impact ionization processes due to $H^*(n) + e$ collisions. The influence of these inverse processes on the $H^*(n)$ atom populations may be characterized by the

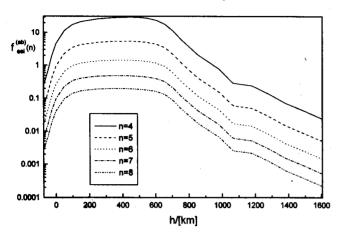


Fig. 3. The behaviour of the quantities $f_{eei}^{(ab)}(n)$, given by Eq. (11), as a function of height h for n = 4 - 8.

corresponding ionization fluxes $I_i^{(ab)}(n)$ and $I_i^{eei}(n)$. The total fluxes $I_{tot}^{(ab)}(n;T)$ and $I_{tot}^{eei}(n;T)$ are than being expressed as

$$I_{tot}^{(ab)}(n;T) = I_r^{(ab)}(n;T) - I_i^{(ab)}(n;T),$$

$$I_{tot}^{eei}(n;T) = I_{r}^{eei}(n;T) - I_{i}^{eei}(n;T).$$

On the basis of Mihajlov et al. (1996), when $T_e = T_a = T$, these total fluxes may be presented in the form

$$I_{tot}^{(ab)}(n;T) = I_{r}^{(ab)}(n;T)[1-\eta(n)],$$

$$I_{tot}^{eei}(n;T) = I_r^{eei}(n;T)[1 - \eta(n)],$$

where, $\eta(n)$ is given by Eq. (5). From here follows that for the considered Solar plasma:

$$f_{eei}^{(ab)}(n) = \frac{I_{tot}^{(ab)}(n, T)}{I_{tot}^{eei}(n, T)}.$$
 (12)

From the definition of $I_{tot}^{(ab)}(n,T)$ and $I_{tot}^{eei}(n,T)$ follows that their values may be also determined with the help of the parameter $\eta(n)$ values presented in Table 2. Moreover, the Table 2 makes it possible to find the limits of layers where the inverse ionization processes start to dominate in comparison with the recombination processes.

Obtained results show that the (1a,b) chemi - recombination processes evidently have an important role in the large region around the temperature minimum in the Solar atmosphere, where they are comparable or dominant in relation to the other recombination processes. Within this range they may be a quite significant factor contributing to the smaller decrease from LTE. Consequently, this shows the necessity of the inclusion of the (1a,b) processes in the modelling of the weakly ionized layers in the Solar atmosphere. For Solar and stellar atmosphere models where $T_e = T_a = T$, the expressions (2-4) for the (1a,b) chemi-recombination processes total rate coefficient $K_r^{(ab)}(n,T)$ may be used. However, for atmosphere models where the equality of

 T_e and T_a is not assumed, the corresponding tables and the general expressions for partially ionized nonequilibrium hydrogen plasma are given in Mihajlov et al. (1996).

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