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Radiative charge exchange in ion–atom collisions at intermediate impact velocities: spectral characteristics and possibilities of experimental studies

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Abstract
The radiative charge exchange processes in $H^+ + H\,(1s)$ and $He^+\,(1s) + H\,(1s^2)$ collisions at intermediate ion–atom impact velocities were treated in this paper from a spectroscopic aspect as new sources of UV and VUV emission. These processes were characterized by the cross-section spectral densities. In the case of hydrogen the corresponding spectral density was calculated for the wavelength λ and impact velocity v in the ranges $1.823\,\text{nm} \leqslant \lambda \leqslant 217.537\,\text{nm}$ and $0.141v_0 \leqslant v \leqslant 1.414v_0$ where v_0 is the atomic unit velocity. Based on these calculations the photon fluxes, generated due to the interaction of weakly ionized low pressure hydrogen plasma with H^+ ion beams, were estimated. It was shown that these fluxes in the UV and VUV domain were strong enough for the spectroscopic measurement. In the case of helium the photon fluxes were estimated in the range $\lambda > 30\,\text{nm}$. It was found that they are smaller than those in the case of hydrogen but still at a substantial level.

The main objective of this work is to emphasize the importance of the radiative charge exchange processes in ion–atom collisions at intermediate impact energies, and to initiate interest in their spectroscopic analysis. These experimental studies can be conducted by measuring the electromagnetic (EM) emission generated in such processes. In turn, obtained experimental data can greatly enhance the studies of various atomic systems. They are not only related to atoms and molecules but also to collisional atomic systems, which can be treated, at least for a short period of time, as quasi-molecular complexes.

Examples of such investigations are atom–atom and atom–excited-atom collision complexes, studied via atomic spectral lines of satellites in gases (Niemax and Pichler 1974, Movre and Pichler 1977, Huennekens and Gallagher 1983, Veza *et al* 1998). The measurement of resonant fluorescence in the absence of thermal atom excitation in considered gases provided necessary data for theoretical studies of several atomic systems. However, such possibilities rarely occur. For this reason those radiative charge exchange processes at intermediate impact velocities which are suitable for spectroscopic analysis are worthy of attention. Based on our previous research in this field (Ermolaev and Mihajlov 1991, henceforth referred to as E&M, Mihajlov *et al* 1997, 2004) we treated here some of the emission charge exchange processes in symmetric ion–atom collisions,

$$A^+ + A \to \varepsilon_\lambda + \begin{cases} A + A^+ \\ A^+ + A, \end{cases} \tag{1}$$

at intermediate impact energies. Here A and A^+ denote the atom and its positive ion in their ground states, and ε_λ is the energy of the photon with the wavelength λ. In E&M, where only the optical part of EM spectra has been considered, A could be any atom with one or two s-electrons out of completed shells (A = H, He, Li, etc). However, here we will consider in detail only the case A = H(1s). The main reason is that the basic method, developed in E&M, can be strictly applied for whole UV and VUV regions in the case of hydrogen only. In addition we briefly considered the case A = He $(1s^2)$, where the mentioned method can be applied in the VUV region without significant loss of accuracy.

In Boggess (1959), the processes (1) with A = H (1s) have been treated as sources of continuous EM emission in plasmas where ion–atom collisions, with impact energies of the order of magnitude of 1 eV, were significant. It was possible to describe these processes within the quasi-static theory (Bates 1951). Astrophysical plasmas were mostly considered (Mihajlov *et al* 1993, 1995, Stancil 1994, Beauchamp *et al* 1997), and also laboratory plasmas in some cases (Ermolaev *et al* 1995).

In the impact energy domain considered, the contribution of processes (1) to the continuous plasma emission is limited to the optical part of the EM spectra only, where their influence cannot be distinguished from other emission processes. Therefore, the direct experimental study of processes (1) through their EM emission is practically impossible. However, an ion beam with intermediate velocities can interact with a weakly ionized plasma. The EM emission generated by the processes (1) in this case will be mostly in the far UV and VUV regions (see Mihajlov *et al* (1997, 2004)), where it will not be masked by the plasma's self-emission. This idea constitutes the general design of such an experiment for the research of EM emission generated in processes (1) at intermediate ion–atom impact velocities.

The cross-section spectral density for the processes (1) at ion–atom impact velocity v, $\mathrm{d}\sigma_A(\lambda, v)/\mathrm{d}\lambda$, was determined by the method developed in E&M. The method is based on quantum electrodynamical theory (Drukarev and Mihajlov 1974) and it is valid under the conditions

$$v \lesssim v_{e;A}, \qquad \varepsilon_\lambda \ll E(v), \tag{2}$$

where $E(v)$ is the ion–atom impact energy in the centre of mass system, and $v_{e;A}$ is the orbital velocity of the electron in an outer shell of the atom A. In the case A = H (1s) we have that $v_{e;H} = v_0$, where $v_0 \cong 2.188 \times 10^8$ cm s^{-1} is the atomic unit of velocity. Within the theory, the electronic state of the collisional $A^+ + A$ system is described by the ground and first excited electronic states of molecular ion A_2^+. These electronic states are denoted by $|1, R\rangle$ and $|2, R\rangle$, where R is the internuclear distance, and $U_1(R)$ and $U_2(R)$ are the corresponding molecular adiabatic terms. The processes (1) in this theory are considered as spontaneous radiative decay of the $|2, R\rangle$ state in the region of R, where the condition

$$U_2(R) > U_1(R) \tag{3}$$

is satisfied. Consequently, the procedure to determine $\mathrm{d}\sigma_A(\lambda, v)/\mathrm{d}\lambda$ requires that the quantities $U_{12}(R)$ and $D_{12}(R)$, defined by relations

$$U_{12}(R) = U_2(R) - U_1(R), \qquad D_{12}(R) = |\langle 1; R|\mathbf{D}|2; R\rangle|, \tag{4}$$

are known functions of R. $\mathbf{D}$ denotes the operator of the total electronic dipole moment of molecular ion A_2^+. In the case of hydrogen, condition (3) is satisfied for all $R > 0$ (see Bates *et al* (1954)); in the case of helium, however, this constraint is satisfied for $R > 0.378a_0$ only (Gupta and Matsen 1967), a_0 being the atomic unit of length.

In the E&M paper, all characteristics of EM emission were treated as functions of the photon's frequency ω. For practical reasons in all our later works these characteristics were treated as functions of λ (Mihajlov *et al* 1993, 1997, 2004). This representation has been adopted in the present paper.

The cross-section density, $\mathrm{d}\sigma_A(\lambda, v)/\mathrm{d}\lambda$, was calculated by the following expressions:

$$\frac{\mathrm{d}\sigma_A(\lambda, v)}{\mathrm{d}\lambda} = \frac{\pi e^2}{3\hbar^3 c}\frac{\sum_{i=1,2} J_i(\lambda, v)}{v^2\lambda^3}, \tag{5}$$

$$J_i(\lambda, v) = 2\pi \int_{\rho_{\min}}^{+\infty} I_i^2(\rho, \lambda, v)\rho\,\mathrm{d}\rho \qquad (i = 1, 2), \tag{6}$$

$$I_1(\rho, \lambda, v) = \int_{-\infty}^{+\infty} \frac{2D_{12}(R(x, \rho))}{eR(x, \rho)} U_{12}(R(x, \rho))x \sin(\Phi(x, \rho))\,\mathrm{d}x, \tag{7}$$

$$I_2(\rho, \lambda, v) = \int_{-\infty}^{+\infty} \frac{2D_{12}(R(x, \rho))}{eR(x, \rho)} U_{12}(R(x, \rho))\rho \cos(\Phi(x, \rho))\,\mathrm{d}x, \tag{8}$$

$$\Phi(x, \rho) = \frac{1}{\hbar v}\int_0^x [\varepsilon_\lambda - U_{12}(R(x', \rho))]\,\mathrm{d}x'. \tag{9}$$

Here e denotes the absolute value of electron charge, $\varepsilon_\lambda = 2\pi\hbar c/\lambda$, $U_{12}(R)$ and $D_{12}(R)$ are defined by relations (4) and $R(x, \rho) = (x^2 + \rho^2)^{1/2}$, where ρ is the impact parameter, and $\rho_{\min} = 0$ in the case of hydrogen and $\rho_{\min} = 0.378a_0$ in the case of helium. In the case of hydrogen, the values for $U_{12}(R)$ and $D_{12}(R)$ were obtained from Bates *et al* (1954), Greenland (1982) and Ramaker and Peek (1972, 1973).

The E&M paper considered only the optical part of EM spectra. Some preliminary calculations in the far UV and VUV regions were performed in Mihajlov *et al* (1997), as well as in Mihajlov *et al* (2004) where the processes (1) were treated from the astrophysical aspect. Here, using the above expressions, we calculated the cross-section density $\mathrm{d}\sigma_{\mathrm{H}}(\lambda, v)/\mathrm{d}\lambda$ in the domains: $1.823\,\mathrm{nm} \leqslant \lambda \leqslant 217.537\,\mathrm{nm}$ and $0.141 \leqslant v/v_0 \leqslant 1.414$. In these regions the photon energy changes from approximately 680 eV to 5.698 eV and the impact energy $E(v)$ changes from 0.25 keV to 25 keV. The results of our calculations of $\mathrm{d}\sigma_H(\lambda, v)/\mathrm{d}\lambda$ are presented in table 1.

Based on these results, we can design the experiments in hydrogen plasmas to check our theoretical models. Consider the weakly ionized hydrogen gas (ionization degree $\sim 10^{-4}$), with H (1s) atom density $N(\mathrm{H})$, in the chamber with volume V. The gas pressure and temperature have to be from regions where the atom density exceeds the densities of all the other components by several orders of magnitude. For example, the gas parameters should be $T = 4\text{–}5 \times 10^3$ K, $p \sim 10^{-4}$ atm. Assume a monoenergetic H^+ ion beam, with the ion density $N(H^+)$ and the velocity $\mathbf{v}$, passing through the ionized gas.

The geometry of such an experiment is schematically shown in figure 1. We assume that the examined photon's flux depends on the angle between $\mathbf{v}$ and the observation direction

Table 1. The differential cross-section $d\sigma_H(\lambda, v)/d\lambda$ in 10^{-25} cm^2 nm^{-1}.

	v/v_0									
λ (nm)	0.141	0.200	0.283	0.447	0.633	0.774	0.894	1.000	1.095	1.414
1.823						0.01	0.01	0.02	0.03	0.12
3.027					0.02	0.06	0.14	0.24	0.35	0.82
4.557				0.03	0.18	0.39	0.62	0.85	1.12	2.15
9.113			0.18	0.79	1.84	2.79	3.67	4.44	5.24	7.94
18.227			4.56	7.40	10.09	11.92	13.54	14.92	16.08	19.58
22.784		4.63	7.46	11.43	14.16	15.96	17.21	18.17	19.00	21.83
26.804		10.30	12.12	14.96	17.01	18.08	18.82	19.47	20.10	22.25
28.480		11.85	13.82	16.20	17.81	18.58	19.16	19.72	20.27	22.05
30.445		13.49	14.57	16.74	18.16	18.76	19.26	19.76	20.24	21.57
35.324		18.89	18.86	19.18	19.03	19.02	19.19	19.41	19.59	19.54
39.721	29.68	24.12	21.87	20.13	18.93	18.57	18.49	18.44	18.33	17.18
45.040	39.27	28.01	23.26	19.82	18.07	17.48	17.12	16.76	16.34	14.28
51.374	47.77	32.71	24.74	19.15	16.84	15.92	15.21	14.52	13.82	11.25
58.896	47.75	35.38	25.31	17.96	15.18	13.89	12.86	11.93	11.08	8.43
67.790	45.65	35.30	24.75	16.42	13.21	11.59	10.35	9.32	8.45	6.07
78.250	40.85	31.90	23.19	14.74	11.10	9.27	7.97	6.98	6.19	4.23
90.487	34.81	26.59	20.26	12.77	8.98	7.12	5.91	5.04	4.40	2.89
104.731	28.88	21.79	16.66	10.54	6.96	5.27	4.24	3.55	3.05	1.95
121.248	23.55	17.37	13.18	8.35	5.21	3.79	2.98	2.46	2.09	1.30
140.363	19.09	13.86	10.15	6.32	3.78	2.67	2.06	1.67	1.41	0.86
162.457	14.25	10.63	7.56	4.60	2.66	1.84	1.40	1.13	0.94	0.57
187.992	10.73	7.92	5.56	3.23	1.83	1.25	0.94	0.75	0.63	0.38
217.537	7.98	5.74	3.97	2.21	1.23	0.84	0.63	0.50	0.42	0.25

only. This angle is denoted by θ in figure 1. We also assume that the mean velocity v_H of H (1s) atoms in the chamber satisfies the condition $v_H \ll v$. Under such conditions the kinetic energy of protons in the ion beam is approximately twice $E(v)$, and it changes from 0.50 keV to 50 keV.

In the described experiment the spectral density of the photon flux, $dF(\lambda, v)/d\lambda$, is given as

$$dF(\lambda, v)/d\lambda = K_H(\lambda, v)N(\mathrm{H})N(\mathrm{H}^+)V\frac{\alpha}{4\pi}\chi(\theta), \tag{10}$$

where $K_H(\lambda, v)$ is the spectral density of the rate coefficient for the processes (1), with $\mathrm{A} = \mathrm{H(1s)}$, defined by

$$K_H(\lambda, v) = v\frac{d\sigma_H(\lambda, v)}{d\lambda}. \tag{11}$$

Figure 2 illustrates the behaviour of this rate coefficient as a function of λ for several values of v. From figure 1 we have the volume $V = lS$, where S is the ion beam cross-section. Note that in equation (10) both densities are given in cm^{-3} and volume in cm^3. The coefficient α denotes a solid angle determined by the geometry of the experiment (see figure 1). The factor $\chi(\theta)$ describes the deviation of the real angular distribution of the examined photons' flux from a uniform one. Although the angular distribution was not treated in E&M, one can show that the factor $\chi(\theta)$ can be expressed within the same procedure by functions J_1 and J_2, defined in equations (6)–(9). Here we will give the final expression for this factor:

$$\chi(\theta) = \frac{3}{2}\left[1 - \frac{1}{2}\frac{2J_1\cos^2(\theta) + J_2\sin^2(\theta)}{J_1 + J_2}\right]. \tag{12}$$

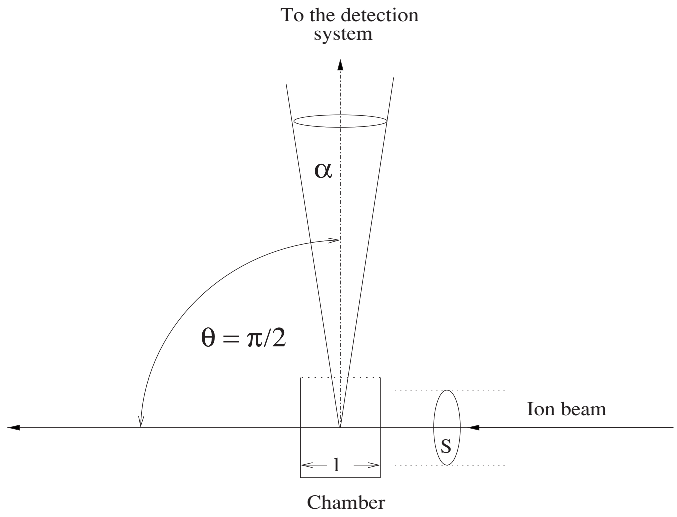

Figure 1. The general design of the experiment.

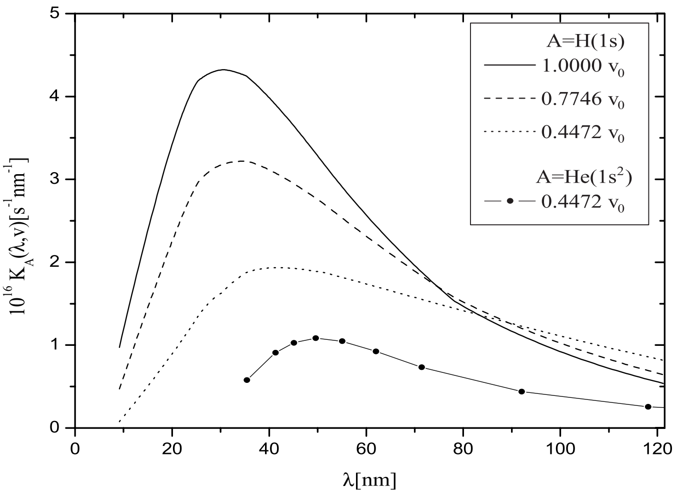

Figure 2. The rate coefficient spectral density $K_A(\lambda, v)$ for chosen impact velocities in the cases of hydrogen and helium.

In order to avoid the influence of the Doppler effect, caused by ion movements, we will assume that the observation direction corresponds to the angle $\theta = \pi/2$, as shown in figure 1. From equation (12) we have

$$\chi(\theta = \pi/2) = \frac{3}{2}\left[1 - \frac{1}{2}\frac{J_2}{J_1 + J_2}\right]. \qquad (13)$$

It follows that $\chi(\theta = \pi/2)$ as a function of v changes between 3/4 and 3/2 only. Our estimation shows that in the entire optical region of λ, the value of $\chi(\theta = \pi/2)$ varies from about 0.80 to 1.10, when the ion beam velocity v changes from $0.0447v_0$ to $1.0000v_0$. In the far UV region the lower value of $\chi(\theta = \pi/2)$ increases.

The chamber length l has to satisfy the condition $l \ll l_{cx}$, where $l_{cx} = [N(\mathrm{H})\sigma_{cx}(v)]^{-1}$ is the mean free path of the proton for the charge exchange process $\mathrm{H}^+ + \mathrm{H}\,(1s) \to \mathrm{H}\,(1s) + \mathrm{H}^+$,

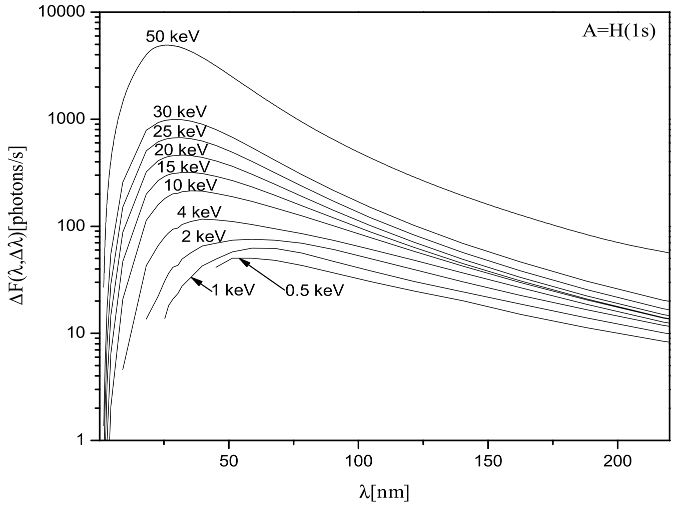

Figure 3. The spectral flux $\Delta F(\lambda, \Delta\lambda)$ for chosen beam energies.

characterized by the cross-section $\sigma_{cx}(v)$. The expression for $\sigma_{cx}(v)$ is given in Janev *et al* (1987) (see also Freeman and Jones (1974)). For $N(\mathrm{H}) = 10^{15}$ cm^{-3} the value of l_{cx} changes from 0.426 cm to 8.930 cm when the value of v changes from $0.141v_0$ to $1.414v_0$.

Now we are able to estimate the flux $\Delta F(\lambda, \Delta\lambda)$ in the interval $(\lambda - \Delta\lambda/2, \lambda + \Delta\lambda/2)$, namely

$$\Delta F(\lambda, \Delta\lambda) \cong \frac{\mathrm{d}F(\lambda, v)}{\mathrm{d}\lambda}\Delta\lambda, \tag{14}$$

where $\mathrm{d}F(\lambda, v)/\mathrm{d}\lambda$ is given by equation (10). To determine $\Delta F(\lambda, \Delta\lambda)$ we have $N(\mathrm{H}^+) = 10^5$ cm^{-3}, $\chi = 0.8$, $l = 0.1l_{cx}$, $S = 1$ cm^2, $\alpha = 0.01$ and $\Delta\lambda = 10$ nm. The results of the calculation for the flux ΔF are shown in figure 3. The curves in this figure correspond to the considered proton beam energies. Note that the curve for $E = 50$ keV reaches its maximum $\Delta F \cong 4900$ photons s^{-1} for $\lambda \cong 28$ nm. As can be seen from figure 3, the values of $\Delta F(\lambda, \Delta\lambda)$ in the region $\lambda < 100$ nm are high enough for successful detection of the examined radiation.

The ion beam–gas interaction causes gas heating in the chamber, which limits the exposure time τ. This is expressed by the condition $W_{int}\tau \ll E(T)$, where W_{int} is the energy per unit of time absorbed by the gas, and $E(T)$ is the internal gas energy at the temperature T. Here we assume that this condition is satisfied if $W_{int}\tau \lesssim 0.1E(T)$. The main contribution to W_{int} comes from the processes of excitation and ionization of hydrogen atoms in $\mathrm{H}^+ + \mathrm{H}$ (1s) collisions. Using the rate coefficients from Janev *et al* (1987), and assuming that the mean energy the atoms obtain in $\mathrm{H}^+ + \mathrm{H}$ (1s) collisions is equal to the ionized energy of the hydrogen atom, we get the maximum exposure time $\tau \sim 1$ s.

In order to estimate the possibility for spectroscopic studies of the processes (1) in the case of helium, we used a similar procedure to determine $\mathrm{d}\sigma_{\mathrm{He}}(\lambda, v)/\mathrm{d}\lambda$ as in the case of hydrogen. The values of $U_{12}(R)$ were taken from Gupta and Matsen (1967), while for $D_{12}(R)$ the approximation from E&M was used. The calculations performed for the same v and λ values in the range $\lambda > 30$ nm showed that the values of the rate coefficient $K_{\mathrm{He}}(\lambda, v)$ in the case of helium are approximately half those in the case of hydrogen. This is shown in figure 2, where the lower curve illustrates the behaviour of $K_{\mathrm{He}}(\lambda, v)$, as a function of λ, for $v = 0.4472v_0$. On the other hand, from figure 3 and equations (10) and (14) calculated with the same atom and ion densities, it follows that the fluxes $\Delta F(\lambda, v)$ in the case of helium are high enough to be measured.

The experimental studies of EM emission generated in processes (1) at intermediate impact energies are important for several reasons. First, at these energies the domain $R \lesssim a_0$ starts to influence the examined EM emission. It gives the possibility of studying the adiabatic terms of non-hydrogen molecular ions in the domains of small R, where they are not well known but their crossing exists. Secondly, the influence of non-adiabatic effects on the behaviour of the system $A^+ + A$ during ion–atom collisions of hydrogen and non-hydrogen atoms can also be investigated. Finally, the radiative charge exchange in non-symmetrical collisions can be of great interest. For example, processes (1) in $He^+(1s) + H(1s)$ collisions, considered in Zygelman *et al* (1989), can be analysed. The collision processes in $H^+ + O$ and $H^+ + N$ systems are important in the interaction of solar wind and higher layers of the Earth's atmosphere.

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References

Bates D R 1951 *Mon. Not. R. Astron. Soc.* **111** 303
Bates D R, Ledsham K and Stewart A L 1954 *Phil. Trans. R. Soc.* A 206
Beauchamp A, Wezemael F and Bergeron P 1997 *Astrophys. J.* **108** 559
Boggess A 1959 *Astrophys. J.* **129** 432
Drukarev G P and Mihajlov A A 1974 *Opt. Spektrosk.* **37** 384
Ermolaev A M and Mihajlov A A 1991 *J. Phys. B: At. Mol. Opt. Phys.* **24** 155 (referred to in the present paper as E&M)
Ermolaev A M, Mihajlov A A, Ignjatović Lj M and Dimitrijević M S 1995 *J. Phys. D: Appl. Phys.* **28** 1047–57
Freeman E L and Jones E M 1974 Atomic collision processes in plasma physics experiments I *UKAEA Report no* CLM-R137 (Abingdon: Culham Laboratory)
Greenland P T 1982 *Phys. Rep.* **81** 133
Gupta B K and Matsen F A 1967 *J. Chem. Phys.* **47** 4860
Huennekens J and Gallagher A 1983 *Phys. Rev.* **27** 185
Janev R K, Langer W D, Evans K Jr and Post D E Jr 1987 *Elementary Processes in Hydrogen–Helium Plasmas* (Berlin: Springer) chapter 3
Mihajlov A A, Dimitrijevic M S and Ignjatovic Lj M 1993 *Astron. Astrophys.* **276** 187
Mihajlov A A, Dimitrijevic M S, Ignjatovic Lj M and Djuric Z 1995 *Astrophys. J.* **454** 420
Mihajlov A A, Ermolaev Lj M and Ignjatović M 2004 *Astron. Astrophys.* **419** 1
Mihajlov A A, Ermolaev A M and Vasilijevic M M 1997 *10th Int. Conf. on Physics of Electronic and Atomic Collisions* Contributed Papers, FR017
Movre M and Pichler G 1977 *J. Phys. B: At. Mol. Phys.* **10** 2631
Niemax K and Pichler G 1974 *J. Phys. B: At. Mol. Phys.* **7** 1204
Niemax K, Movre M and Pichler G 1979 *J. Phys. B: At. Mol. Phys.* **12** 3503
Ramaker D and Peek J 1972 *J. Phys. B: At. Mol. Phys.* **5** 2175
Ramaker D and Peek J 1973 *At. Data* **5** 167
Stancil P C 1994 *Astrophys. J.* **430** 360
Veza D, Beuc R, Milosevic S and Pichler G 1998 *Eur. Phys. J.* D **2** 45
Zygelman B, Dalgarno A, Kimura M and Lane N F 1989 *Phys. Rev.* A **40** 23–40