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Line emission from charge transfer with atomic hydrogen at thermal energies

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A list is assembled of the emission lines produced by the charge transfer of doubly and trebly charged ions of carbon, nitrogen, oxygen, and neon in collision at low energies with atomic hydrogen. Rate coefficients of 2.0×10^{-9} cm^{3}s^{-1} for the process $O^{3+}+H\rightarrow O^{2+}(2p\,3p,\,^1P)+H^+$ and of 2.1×10^{-9} cm^{3}s^{-1} for the process $O^{3+}+H\rightarrow O^{2+}(2p\,3p,\,^3D_1)$ at 1 eV are obtained by comparing observations of planetary nebulae with detailed models.

I. INTRODUCTION

Charge transfer of multiply charged ions in collisions with neutral hydrogen or deuterium atoms is an important process in plasma heating by neutral particle beam injection[1] and in the transport and radiation losses of impurity ions.[2] The emissions resulting from charge transfer of energetic ions have been used as a probe of the conditions in several tokamak plasmas.[3–6] Emission lines may be produced with high efficiency also in charge transfer at thermal energies.[7] Detailed quantal calculations of the cross sections for doubly and trebly charged ions of carbon, nitrogen, oxygen, and neon and for doubly charged ions of silicon and sulfur undergoing charge transfer in collisions at low impact energies with atomic hydrogen have been carried out recently.[8–20] Low-energy collisions of more highly stripped carbon ions have also been investigated.[18,21] Other systems have been studied using the Landau-Zener approximation and an extensive tabulation has been assembled by Butler and Dalgarno.[22] The theoretical total charge transfer cross sections agree to within experimental error with the measurements on C^{3+} ions[23] and to within a factor of 2 with the measurements on O^{3+} ions.[24,25] The theoretical studies do not take full account of the effects of momentum translation and rotational coupling, and are restricted to a small number of molecular states constructed from a limited atomic basis set. The experiments are affected by the presence of metastable ions.

The theoretical analyses show that the low-energy charge transfer of multiply charged ions occurs in several channels whose end products are ions in specific excited states. The contribution of any particular channel varies with impact energy. A deeper test of the theory and a critical assessment of the role of metastable ions would be provided by measurements of the individual channel cross sections which may be made by detection of the spectral lines emitted by the excited product ions[26–29] and by energy-gain spectroscopy.[29–32]

We present here a list of the emission lines of ions of C, N, O, and Ne which are predicted to appear as a result of low-energy charge transfer and which may be useful as diagnostic probes of the processes and of the physical environments in which they take place. Some of the lines are observed in the spectra of astrophysical objects like planetary nebulae. We construct models of planetary nebulae which demonstrate that several emission lines of O^{2+} are produced preferentially by charge transfer recombination of O^{3+} ions in collision with H atoms and we derive quantitative estimates of the individual channel charge transfer rate coefficients at temperatures near 1 eV.

II. EMISSION LINES

The excited states populated by low-energy charge transfer of doubly or trebly charged ions of C, N, O, and Ne with H atoms[15,17,20] and the wavelength span of the resulting multiplet emission lines are listed in Table I.

TABLE I. Excited states populated by charge transfer recombination and the resulting allowed emission line wavelengths (in nm).

State	Wavelengths
$C^+(2s\,2p^2,\,^2D)$	133.45–133.57
$N^+(2s\,2p^3,\,^3D^o)$	108.40–108.57
$O^+(2s\,2p^4,\,^4P)$	83.28–83.45
$C^{2+}(2p^2,\,^1S)$	124.7 (97.70)
$C^{2+}(2s\,3s,\,^3S)$	53.81–53.83
$N^{2+}(2s^2 3s,\,^2S)$	45.19–45.22
$O^{2+}(2s^2 2p\,3s,\,^3P^o)$	37.38–37.44
$O^{2+}(2s^2 2p\,3p,\,^3D)$	375.47–381.10 (37.38–37.44)
	65.96–64.17 (70.05–70.23)
$O^{2+}(2s^2 2p\,3p,\,^3S)$	329.94–344.07 (37.38–37.44)
	64.44–64.45 (70.05–70.23)
$O^{2+}(2s^2 2p\,3s,\,^1P^o)$	39.56, 43.50
$O^{2+}(2s^2 2p\,3p,\,^1P)$	559.24 (39.56, 43.50)
	96.24 (59.96)
	124.23 (52.58, 59.78)
$Ne^{2+}(2p^3 3p,\,^5P)$	259.00–259.57
$Ne^{2+}(2p^3 3s,\,^3D^o)$	28.31–28.39
$Ne^{2+}(2p^3 3p,\,^3P)$	2755. 9–2802.1 (28.31–28.39)
	267.79–267.86 (31.30–31.39)
	65.58–65.98 (48.73–49.17)

Table I also includes in parentheses the wavelengths of the additional lines produced by cascading in allowed transitions. Cascading also populates $C^{2+}(2s\,2p,\,{}^3P)$ which may decay by forbidden transitions at 190.7 and 190.9 nm, $O^{2+}(2p^2,\,{}^1S)$ and $O^{2+}(2p^2,\,{}^1D)$ which may decay by forbidden transitions near 436.3, 500.7, 233.2, and 495.9 nm,[33] and $Ne^{2+}(2p^3 3s,\,{}^5S^o)$, which may decay by a forbidden transition at 31.83 nm.

Most of the lines appear in the ultraviolet or extreme ultraviolet region of the spectrum, and the reactions are possible candidates for ultraviolet lasers. Of particular interest as diagnostic probes are the singlet line of O^{2+} at 559.24 nm (Ref. 17) and the triplet array between 300 and 380 nm.[34] The lines have been observed in planetary nebulae.

III. ASTROPHYSICAL PLASMAS

Multiply charged ions may coexist with neutral material in astrophysical plasmas produced by nonthermal sources of ionization. The excited levels of multiply charged ions have large excitation energies and they are not populated efficiently by impact with thermal electrons. With the possible exception of the singly charged species, electron-impact excitation of the levels listed in Table I is negligible in plasmas with temperatures of the order of 1 eV and charge transfer may be the major excitation mechanism.

The upper level of the singlet line of O^{2+} at 559.24 nm lies at an energy of 36 eV above the ground state of the ion. The line is seen in most high excitation nebulae which are distinguished from low excitation nebulae by the presence in the spectrum of strong recombination lines of He^+ and, in particular, the line at 468.6 nm. In the tabulations of Aller and Walker[35] of the spectral line intensities observed in nebulae, the intensity $I(559.2)$ of the line at 449.2 nm expressed as the ratio $I(559.2)/I(H\beta)$, where $I(H\beta)$ is the intensity of the hydrogen $H\beta$ line, is about 1.8×10^{-3} for 13 objects in which the He^+ line intensity ratio $I(4686)/I(H\beta)$ exceeds 0.1, but the 559.2-nm line is absent in five objects with lesser He^+ emission. Because it is produced by radiative recombination, the presence of the He^+ 468.6-nm line indicates the existence of a zone of He^{2+} ions in the nebulae. The ionization potentials of He^+ and O^{2+} are similar with values of 54.403 and 54.934 eV, respectively, and the He^{2+} zone is the site of the O^{3+} ions. Thus, the observational data suggest that emission of the 559.2-nm line of O^{2+} is associated with O^{3+} and provide qualitative support for the identification of either charge transfer or radiative and dielectronic recombination as the population mechanism. There appears to be no accessible singlet autoionizing level of O^{2+} so that dielectronic recombination is unlikely to be significant. Quantitative support for the charge transfer mechanism may be obtained from construction of models of the emitting plasmas.

It is convenient to characterize the ionization distribution of astrophysical nebulae by mean ionization fractions. Writing

$$X(Y^{m+})=n(Y^{m+})/n_Y\ ,$$

where n_Y is the total number of Y nuclei, we integrate over the nebular volume to obtain the mean fractional ionization

$$\langle X(Y^{m+})\rangle=\frac{\int X(Y^{m+})n_e dV}{\int n_e dV}\ ,$$

where n_e is the electron density.

Let α_{eff} be the effective recombination rate coefficient producing the $H\beta$ line and let k_{eff} be the effective charge transfer rate coefficient producing the 559.24 line. The branching ratio for the emission of 559.2 nm by the excited ${}^1P$ level of O^{2+} is 0.225 (Ref. 33) so that $k_{\text{eff}}=0.225k({}^1P)$, where $k({}^1P)$ is the rate coefficient for charge transfer into the ${}^1P$ state. Then integrating over the nebular volume, we obtain the intensity ratio

$$\frac{I(559.2)}{I(H\beta)}=\frac{h\nu(559.2)}{h\nu(H\beta)}\frac{\int k_{\text{eff}}n(H)n(O^{3+})dV}{\int \alpha_{\text{eff}}n_e n(H^+)dV}\ ,$$

where the ν's are frequencies and the n's are number densities.

The models show little variation of temperature through the nebulae, so that we may write

$$\frac{I(559.2)}{I(H\beta)}=\frac{h\nu(559.2)}{h\nu(H\beta)}\frac{k_{\text{eff}}}{\alpha_{\text{eff}}}\frac{\int n(H)n(O^{3+})dV}{\int n_e n(H^+)dV}\ .$$

Then for a nebula of uniform density,

$$\frac{I(559.2)}{I(H\beta)}=\frac{h\nu(559.2)k_{\text{eff}}}{h\nu(H\beta)\alpha_{\text{eff}}}\frac{n_0}{n_H}\frac{\xi_H(O^{3+})}{\langle X(H^+)\rangle}\ ,$$

where

$$\xi_H(O^{3+})=\int X(O^{3+})n(H)dV\Big/\int n_e dV\ .$$

Shields *et al.*[36] have constructed a detailed model of the high excitation planetary nebula NGC-2440 for which ionization results from absorption of photons from a high-frequency central stellar source and is removed through radiative and dielectronic recombination and charge transfer. The model successfully reproduces a wide range of spectral data. Using the model we have calculated the parameters $\langle X(Y^{m+})\rangle$ and $\xi_H(Y^{m+})$ and the results for hydrogen, helium, carbon, nitrogen, oxygen, and neon are shown in Tables II and III.

The observed ratio $I(559.2)/I(H\beta)$ for NGC-2440 is 1.4×10^{-3}. The mean temperature of NGC-2440 is 13 000 K. At 13 000K $\alpha_{\text{eff}}=2.6\times10^{-14}\ \text{cm}^3\,\text{s}^{-1}$ (Ref. 37) and we derive for $k({}^1P)$ an empirical value of $2.0\times10^{-9}\ \text{cm}^3\,\text{s}^{-1}$. The theoretical value is $1.6\times10^{-9}\ \text{cm}^3\,\text{s}^{-1}$.[12]

Emission at λ559.2 nm is also detected in the planetary nebula NGC-7027. In one model a filamentary structure was adopted with a total density of $6\times10^4\ \text{cm}^{-3}$ and a volume filling factor of 0.09, and in a second model a total density of $10^5\ \text{cm}^{-3}$ was assumed to occupy a shell between radii of 4.5×10^{16} and 6.6×10^{16} cm.[38] The observed intensity ratio $I(559.2)/I(H\beta)$, corrected for reddening, is 1.2×10^{-3}. Using $k({}^1P)=1.6\times10^{-9}\ \text{cm}^3\,\text{s}^{-1}$, the predicted ratios are 2.0×10^{-3} for the filamentary structure and 1.2×10^{-3} for the shell geometry.

The closeness of the agreement between the models of

TABLE II. Ionization parameters $\langle X(Y^{m+})\rangle$ in NGC-2440.

Y/m	0	1	2	3	4	5	6
H	0.14	0.86					
He	0.077	0.52	0.40				
C	0.003	0.28	0.44	0.16	0.13		
N	0.066	0.27	0.38	0.17	0.067	0.040	
O	0.13	0.18	0.46	0.091	0.099	0.035	0.006
Ne	0.022	0.064	0.61	0.14	0.099	0.055	0.006

NGC-2440 and NGC-7027 and the observations is partly fortuitous, but it does establish that charge transfer of O^{3+} with H leads to a significant population of excited $O^{2+}(2p\,3p\;^1P)$ ions and it suggests that the calculated rate coefficient for capture into the $(2p\,3p\;^1P)$ state is correct at temperatures near 1 eV to within a factor of 2.

Emission lines originating in the $(2p\,3p\;^3S)$, $(2p\,3p\;^3D)$, and $(2p\,3s\;^3P^o)$ levels of O^{2+} are observed at wavelengths between 302 and 381 nm in a wide range of astrophysical objects. Their interpretation is less straightforward because the excited states are also populated by the Bowen fluorescence mechanism, initiated by the absorption of the He^+ resonance line at 30.380 nm by O^{2+} into the $(2p\,3d\;^3P_2^o)$ state.[39] For most of the triplet emission lines in most of the sources, pumping by the He^+ line is the major population mechanism, but it fails to explain the measured intensities of lines at 377.4 and 375.7 nm produced in planetary nebulae[40] which arise from the $(2p\,3p\;^3D_1)$ fine-structure state.

If it is assumed that charge transfer of O^{3+} with H is the main excitation mechanism for $O^{2+}(2p\,3p\;^3D_1)$, a rate coefficient for the process may be derived from a comparison of the intensities of the 377.4- and 375.7-nm lines with that of the 559.2-nm line in the same object.[34] From observations of the planetary nebulae NGC-7662 and PK-86-801, we derive a rate coefficient of 2.1×10^{-9} $cm^3\,s^{-1}$ for the charge transfer reaction

$$O^{3+}(2s^22p)+H\rightarrow O^{2+}(2s^22p\,3p,\,^3D_1)+H^+\ .$$

No calculations of charge transfer into specific fine-structure levels have been reported. The theoretical value for capture into all the ^3D_J levels is 6.2×10^{-9} $cm^3\,s^{-1}$ at 10^4 K.[17]

Although the derived rate coefficient is consistent with the quantal calculations of charge transfer, triplet autoionizing levels of O^{2+} exist[41] which may decay radiatively to the $(2s^22p\,3p,\,^3D_1)$ level and we cannot exclude the possibility of a contribution from dielectronic recombination. The atomic data needed to predict the intensity that may result from dielectronic recombination are not available.

Of the other lines produced by charge transfer, the forbidden cascade lines at 190.7 and 190.9 nm of C^{2+}, though observed in many kinds of astrophysical objects, are excited mainly by electron collisions and the lines of C^+ near 133.5 nm and of C^{2+} at 124.7 nm are excited mainly by dielectronic recombination.[42–44] The lines of Ne^{2+} near 259 and 268 nm lie in the wavelength range covered by the International Ultraviolet Explorer telescope.[45] For the planetary nebula NGC-2440, our model gives an intensity relative to Hβ of 2.2×10^{-2} for the 259-nm lines.

The intensity of the 268-nm lines depends upon the unknown branching ratios of the transitions from the $(2p^33p\;^3P)$ state to the $(2p^33s\;^3D^o)$, $(2p^33p\;^3S^o)$, and $(2s\,2p^5\;^3P^o)$ states. With the arbitrary choice of 0.5 for the branching ratio for the transition to the $(2p^33p\;^3S^o)$ state, the intensity is 1.8×10^{-2}. The lines are predicted to be stronger than the oxygen lines with intensities not much below those of other lines near 260 nm which have been detected.[36]

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TABLE III. Charge transfer emission measures $\xi_H(Y^{m+})$ for NGC-2440. "9.0(−3)" is a shorthand for 9.0×10^{-3}.

Y/m	1	2	3	4	5
H	0.10				
He	0.31	9.0(−3)			
C	0.00	0.018	7.8(−4)	1.6(−4)	2.4(−9)
N	0.48	7.1(−3)	8.4(−4)	1.1(−4)	2.8(−5)
O	0.081	9.1(−3)	2.2(−4)	1.3(−4)	2.9(−5)
Ne	0.98	0.36	5.1(−4)	1.5(−4)	4.8(−5)

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