Revista Mexicana de Astronomía y Astrofísica, **32**, 69–73 (1996)

SOFT X IRRADIATION OF LOW DENSITY PLASMAS: O III AND O IV LINE EMISSION

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Received 1995 November 13; accepted 1996 May 24

RESUMEN

Los fotones energéticos (0.55–2 keV) producen eficientemente hoyos 1s y 1s+2p de iones de oxígeno, respectivamente, mediante los procesos de ionización sencilla y el de liberación de oxígeno neutro. Se estima que este último efecto excede en un 25% al primero, alcanzando su eficiencia total arriba de 0.8 keV. El decaimiento Auger de estos iones con hoyo 1s producen estados excitados en O III y O IV, dando lugar a líneas ópticas y ultravioleta de O III y O IV. En plasmas de baja densidad sometidos a una fuente de fotones enérgicos con un exceso de rayos X suaves, menores a 1 keV, esta producción directa de estados excitados debe tomarse en cuenta antes de usar las líneas [O III] y O III] como indicadores de T_e o N_e debido a que las líneas $\lambda\lambda$4960, 5008 y $\lambda\lambda$1661, 1667 están indirectamente afectadas por el decaimiento Auger. El decaimiento Auger y las tasas de radiación para el ión residual O IV se presentan en una forma conveniente para evaluar las tasas efectivas y las intensidades relativas en las líneas de O III y O IV emitidas en plasmas de baja densidad, bajo irradiación X suave.

ABSTRACT

Energetic 0.55–2 keV photons produce efficiently 1s–hole and 1s+2p–hole oxygen ions by single ionization and shake off processes of neutral oxygen, respectively. This last effect is estimated to exceed 25 percent of the single one, reaching its full efficiency at above 0.8 keV. Auger decays of these 1s–hole ions will produce O III and O IV excited states giving rise to O III and O IV ultraviolet and optical lines. In low density plasmas submitted to a source of energetic photons with soft X-ray excess below 1 keV this *direct* production of excited states must be taken into account before using [O III] and O III] lines as indicators of T_e or N_e since $\lambda\lambda$4960, 5008, $\lambda\lambda$1661, 1667 are indirectly affected by Auger decay. Auger and radiative rates for O IV residual ion are presented in a convenient form for evaluating effective Auger rates and relative intensities for O III and O IV lines produced by low density plasmas under soft X irradiation.

Key words: **ATOMIC DATA — X–RAYS – GENERAL**

1. INTRODUCTION

In the early seventies Weisheit & Dalgarno (1972) reported equivalent widths of carbon absorption lines for several models of H I regions. Following K-shell ionization, Auger processes dominate largely radiative K_α decay for low-Z elements (Bambynek et al. 1972) thus affecting the ionization balance. Later, the cases of C, N, O were further investigated in the interstellar gas ionized by a diffuse X-ray background showing energy excess in the 0.15–0.50 keV range (Weisheit 1973). Heavier elements such as Mg, Al, Si and S were treated by the same author (Weisheit 1974) with a special emphasis on Si ionization balance. McAlpine (1974) noted the significance of Auger electron removal for QSO and Seyfert galaxy line-emitting regions. Osterbrock (1989) describing the Active Galactic Nuclei where energetic photons around 1 keV abound (see Mushotzsky, Done, & Pounds 1993), emphasized the case of oxygen since the [O III] nebullium lines are the best indicators of T_e. Kaslahn (1975) and Shapiro & Bahcall (1981) stressed the possibility of producing UV and optical lines from X irradiation of plasmas. Emission of 2s–2p lines in lithium-like ions due to the Auger decay selective production of $1s^22p$ states from $1s2s^22p$ radiationless transition was considered by Kallman & McCray (1982). Recently Kaastra & Mewe (1993) calculated the probability distribution for the number of ejected electrons following innershell ionization, as well as the X-ray production probability of all atoms and ions from Be to Zn. Their goal was to include the main process (single innershell photoionization followed by Auger decay) in steady-state calculations where photoionization by energetic photons plays a crucial role i.e., thin, hot plasmas such as BO star envelopes, stellar coronae, supernova remnants and active galactic nuclei.

In the seventies also, Krause, Carlson, and Moddeman at Oak Ridge National Laboratories (cf., Krause 1971; Krause, Carlson, & Moddeman 1971; Carlson, Krause, & Moddeman 1971) studied the neon 1s photoionization process due to irradiation of a gas target by characteristic X-rays (K_α Mg and Al: 1253.6 and 1486.6 eV; Ne 1s potential: 870 eV). They found a high probability of simultaneous excitation (shake up) and ionization (shake off) of a second electron in the same atom respectively 8.1 and 13.8 percent relative to *all processes* (see also Wuilleumier & Krause 1974). Morever, experimental evidence for double electron emission in Auger process, i.e., simultaneous ejection of two electrons in the Auger process itself, was shown by Carlson & Krause (1965). This Ne^{+++} production does not exceed 6.5 percent relative to all processes. Subsequent theories showed a good agreement with these experiments (Kelly 1975; Petrini 1982 for Auger rates; Carlson & Nestor 1973 for shake off; Martin & Shirley 1976 for shake up). The studies by Åberg (1969) on shake up and shake off for light ions and atoms, down to fluorine, make evident the *increasing* importance of these processes with *decreasing* atomic charge and the decrease of shake off with the asymptotic charge of the target ion (still significant for the first ions). These results mean that the C, N, and O atoms and ions will be significantly affected by the shake off process (roughly 35 to 25 percent of single photoionization). Regarding oxygen, experimental and theoretical results are scarce (Caldwell & Krause 1993; Caldwell et al. 1994; Petrini & de Araújo 1994). Moreover, even admitting that in low density plasmas most atoms or ions overpopulate the ground state and noting that both theory and experiment show the 1s-hole $^2P^e$ and $^4P^e$ states to be populated according to their statistical weights (s.w. thereafter), we are still faced with difficulties in estimating the relative populations of *shaken up* O II and *shaken off* O III terms (1s-hole terms, see Table 1). Recently Petrini & de Araùjo (1994) and Petrini & Farias (1994) limiting somewhat their investigations, carried out some relative soft X-ray line intensities of O III as well as some Ne III and IV relative line intensities using the ORNL data. For Ne, 99% of the single ionization reaches *excited* residual Ne III terms and for O III only 45% is obtained. However no attention was paid to nebullium and neon forbidden lines. Aldrovandi & Gruenwald (1985) treated the [O III] line emission in active galactic nuclei but with limited information on the complete innershell photoionization process. In this paper, before tackling other elements (atoms and ions), like carbon, nitrogen, neon, sulfur and argon (for these last ones Coster-Kronig rates will be considered), we consider first, the production of [O III] lines, and in addition we give the Auger rates of the $1s2s^22p^3$ O III terms and the radiative rates plus wavelengths for the residual O IV terms. These O IV terms, given in Table 1, are created with different probabilities, whether originating from shake off from O I or from single 1s-ionization from the O II ^4S ground term. We present some relative line intensities emitted by low density plasmas undergoing soft X irradiation.

2. RESULTS AND DISCUSSION

2.1. [O III] and O III] Line Intensities

The experimental Auger spectrum, besides the $1s2s^22p^4$ ^2P and ^4P main contributions, contains lines originating mainly from $1s2s^22p^3np$ ^2P and ^4P (n = 3,4) Auger decays due to the shake up processes 2p→np. These 1s-hole states give rise to Auger lines related to $2s^22pnp$, $2s2p^2np$ and $2p^3np$ O III states. Caldwell et al. (1994) give a relative value of roughly 6% for the shake up process. In our work shake up and double Auger processes affect de facto the O III and O IV relative populations by a few percent. We retain the experimental results (see Table 1 of Petrini & de Araújo 1994) but the $i = 8$ and 9 results (0.58(5);0.0) are changed to (0.50;0.08) to agree with our ^2P calculated values (0.495;0.087). By using these experimental results we obtain for the relative direct or indirect production rates to ^1D, ^1S and $^5S^o$ respectively 0.028 (with radiative cascade from $i = 9$), 0.001, and 0.022. The lowest ^1S state is weakly populated due to the low branching ratio of 3←9 (see Table 2 of Petrini & de Araújo 1994). Consequently $R_1 = \epsilon(\lambda\lambda 1661, 1667)/\epsilon(\lambda\lambda 4960, 5008) \simeq$

TABLE 1

PARTIAL AUGER RATES FOR $1s2s^22p^3$ TERMS

	$^2P^o(1)$	$^4P^e(2)$	$^2D^e(2)$	$^2S^e(2)$	$^2P^e(2)$	$^4S^o(3)$	$^2D^o(3)$	$^2P^o(3)$	Width (10^{-4} a.u.)	e.e.e. (eV)
$^3S^o$	...	3.28 p	...	...	5.72 p	12.10 s	0.22 d	...	21.32	485
$^5S^o$	...	22.86 p	...	...	...	9.00 s	...	...	31.86	479
$^1P^o$	11.00 d	...	0.05 f	0.06 p	10.30 p	...	1.61 d	0.14 d	40.63	490
	6.75 s	...	...	...	...	...	...	10.71 s	...	...
$^3P^o$	11.87 d	2.19 p	0.12 f	4.41 p	4.10 p	...	1.62 d	9.28 s	46.34	486
	6.51 s	...	6.22 p	...	...	...	...	...	...	...
$^1D^o$	20.28 d	...	0.05 f	...	0.20 f	...	0.16 d	1.02 d	43.32	488
	...	...	0.07 p	...	9.98 p	...	11.56 s	...	...	...
$^3D^o$	20.39 d	2.19 p	0.14 f	...	0.17 f	...	9.91 s	1.00 d	48.66	485
	...	...	10.92 p	...	3.88 p	...	...	...	...	...

First column: $1s2s^22p^3$ terms. Two last columns respectively: total Auger width and ejected electron energy with respect to the O IV ground state. Other columns: partial Auger rates, 22.86 p means 22.86 10^{-4} a.u. for channel $^4P^e$, $l = 1$, where 1 a.u. = 4.134×10^{16} s^{-1}. Only channels with width coefficients larger than 0.05 are shown. (1), (2) and (3) refer to configurations $1s^22s^22p$, $1s^22s2p^2$ and $1s^22s2p^3$, respectively.

2.3 and $R_2 = \epsilon(\lambda4363)/\epsilon(\lambda\lambda4960, 5008) \simeq 10^{-3}$. Nussbaumer & Storey (1981) have presented tables of steady-state relative populations of $^1D_2$, $^1S_0$ and $^5S_2$ states for T_e in the range of 7 500–40 000 K and $\log N_e$ in the range of 2.0–12.5 in [cm^{-3}]. Their Fig. 2 which is reproduced here as Figure 1 shows the ratios of some UV line emissivities. For low density medium the arrow indicates the segment of increasing temperatures to be considered. Using our R_1 and R_2 values we have a cross indicated in Figure 1. The Auger effect tends to *increase* the temperature if R_1 is considered. Note that the relative productions of $i = 10$, 5 and 7 are respectively 0.12, 0.25 and 0.02 which indicate a relatively strong emissivity of $\lambda834.50$ and an emissivity ratio $\lambda610.4/\lambda599.6 \simeq 6.2$.

2.2. O IV Line Production

We use the University College London Codes to calculate *partial* Auger rates from the O III $1s2s^22p^3$ states i.e., $^3S^o$, $^5S^o$, $^1P^o$, $^3P^o$, $^1D^o$ and $^3D^o$ terms. The residual O IV terms of the basic configurations $1s^22s^22p$, $1s^22s2p^2$ and $1s^22p^3$ are shown in Figure 2. In order to avoid unnecessary developments of our method we refer the reader to our previous article on boron (Petrini 1981). Table 1 presents these partial Auger rates from each initial 1s-hole term. If we consider these O III 1s-hole terms equally produced, we find that 71.3% of Auger decay ends up as O IV residual *excited* states. For the s.w. distribution the previous number is now 66.3. Figure 2 shows the O IV residual ion terms with the corresponding allowed transition probabilities and wavelengths. For each residual term two numbers appear on the right and are relative *direct* production rates and refer respectively to initial O III terms created with $\omega_i = 1$ and $\omega_i = (2L+1)(2S+1)$. Note that if the single ionization of O II $^4S^o$ ground state is responsible for the O IV term creation one of the most intense line is $\lambda625.41$ since the $^4S^o$ absorbs 39% of the total O IV Auger production. The most intense line is then $\lambda1400$ with a reinforced production rate of 0.89.

For defining *effective* Auger rates for O III and O IV states originating from the O I ground state, we have to estimate the relative importance of the shake off process with respect to the single K-ionization. The theoretical works of Åberg (1969) and the experimental data of Löw et al. (1984) lead to a value superior to 30%. The effective relative production is very dependent on the 0.5–1 keV range behaviour of the incident radiation (above 1 keV the full regime shake off process acts which implies that a X-ray source with a pronounced peak at 1 keV is a perfect choice). We choose the production rate of O IV to be 20% of O III. Although the s.w. rule applies for the $1s2s^22p^4$ ^2P and ^4P term production (Caldwell et al. 1994), a still controversial question is the respect of this rule for the $1s2s^22p^3$ term production. We side here

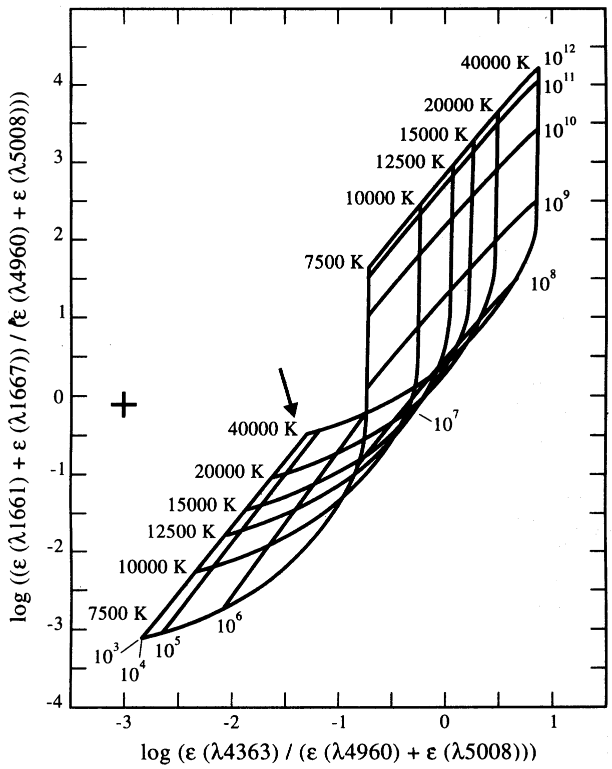

Fig. 1. Ratio of emissivities of the UV intercombination lines λλ1661, 1667 (^{3}P – ^{5}S^o) to the forbidden lines λλ4960, 5008 (^{3}P – ^{1}D) plotted against the corresponding ratio of the forbidden line λ4363 (^{3}P – ^{1}S) to the lines λλ4960, 5008 as a function of T_e and N_e (from Nussbaumer & Storey 1981). The cross is obtained from this work (see *2.1*), the arrow indicates the lowest N_e density (10^3 cm^{-3}).

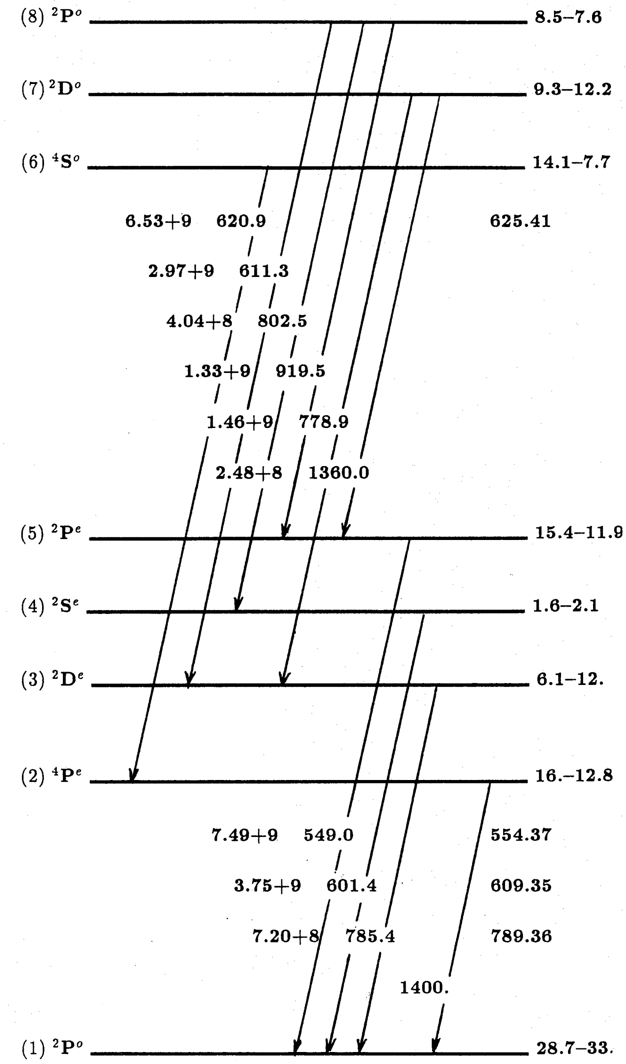

Fig. 2. O IV terms related to configurations 1s^{2}2s^{2}2p, 1s^{2}2s2p^2 and 1s^{2}2p^3. Wavelengths and radiative rates for allowed transitions are given (O.P. Data Bank, see text). 6.53+9 = 6.53 10^9 s^{-1}. On the right side for each term the Auger relative rates are given, the two numbers that appear were derived assuming equal population for initial 1s-hole terms or statistical weight populations, respectively. Some wavelengths from Wiese, Smith, & Glennon (1966) are also given on the right hand side.

with the s.w. distribution. Consequently for low T_e, N_e values the O IV λ778.9/λ789.36 relative intensity is 0.38 due to radiative cascade amplifications to (3) and the O III λ834.5/OIVλ789.36 relative intensity is 4.3. In the same way we obtain $\epsilon(\lambda1400)/\epsilon(\lambda1360) \simeq 11$. The λ610.4 O III line originating from the 1s^{2}2p^4 ^{3}P state absorbs 12.5% of the Auger decay and can be compared with the O IV λ625.4 line (both originating from upper configurations). We obtain O III $\epsilon(\lambda610.4)$/OIV$\epsilon(\lambda625.41) \simeq 1.7$.

3. CONCLUSIONS

In this work we have shown how the K–LL+KL–LLL mechanism (complete innershell ionization processes + Auger decays) can efficiently act to populate excited states of twice and three times ionized oxygen. But, if this mechanism affects the ionization equilibrium of oxygen species it does not affect really the relative excited states populations of O I and O II since Auger processes following K-shell ionization generate only twice and three times ionized ions (fluorescence yields are around 0.01). The ORNL experiments on atomic oxygen were conducted with a 590 eV photon source insufficient for fully inducing the shake off process. Experiments with larger photon energies are needed since the confirmation of the high shake off probability for atomic oxygen, theoretically predicted by Åberg (1969) for light atoms, would guarantee the importance of this effect for carbon and nitrogen atoms and ions. These processes are generally marginal in the physics of planetary nebulae but they participate on the C, N, O line emission in ionized regions surrounding supersoft X-ray sources. For example in the standard model of Rappaport et al. (1994) the external region undergoes a substantial and dominating flux of 200–800 eV photons. Since the neutral species dominates, there exists the possibility of observing O III and IV lines (UV and optical) and certainly C III and C IV lines. Production of Ne IV, V, VI and O IV, V, VI by the same complex mechanism but acting on ionized targets will be considered elsewhere (since Ne and O exist often in their multi-ionized forms). Tables of Auger rates for all terms of the configuration $1s2s^22p^3$ and A_{ij} for O IV soft UV lines (from Opacity Project data bank, Seaton et al. 1992) are presented in a useful form. Our future goal is to carry out calculations or estimations on shake up and shake off processes for light atoms and ions, as well as calculations of Auger and Coster-Kronig partial rates since these processes compete with electronic excitation for producing highly excited states.

The authors thank J.A. Tully, T. Åberg and the referee for their patient comments. They also thank G. Urbach at Centre National Universitaire Sud de Calcul at Montpellier for his comprehensive assistance.

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