Beyond simple ionization & radiative recombination

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January 30, 2023

The (electron or photon) ionization of hydrogen is dealt at some length in ISM classes. However, hydrogen, by having only one electron, is atypical. Ionization of atoms/ions with multiple electrons is radically different from that of hydrogen. In particular, for multiple electron atoms and ions there are many pathways for ionization.Compare the next two figures to appreciate this point. Note that apart from that for hydrogen the photo-ionization cross-sections are heavily smoothed.

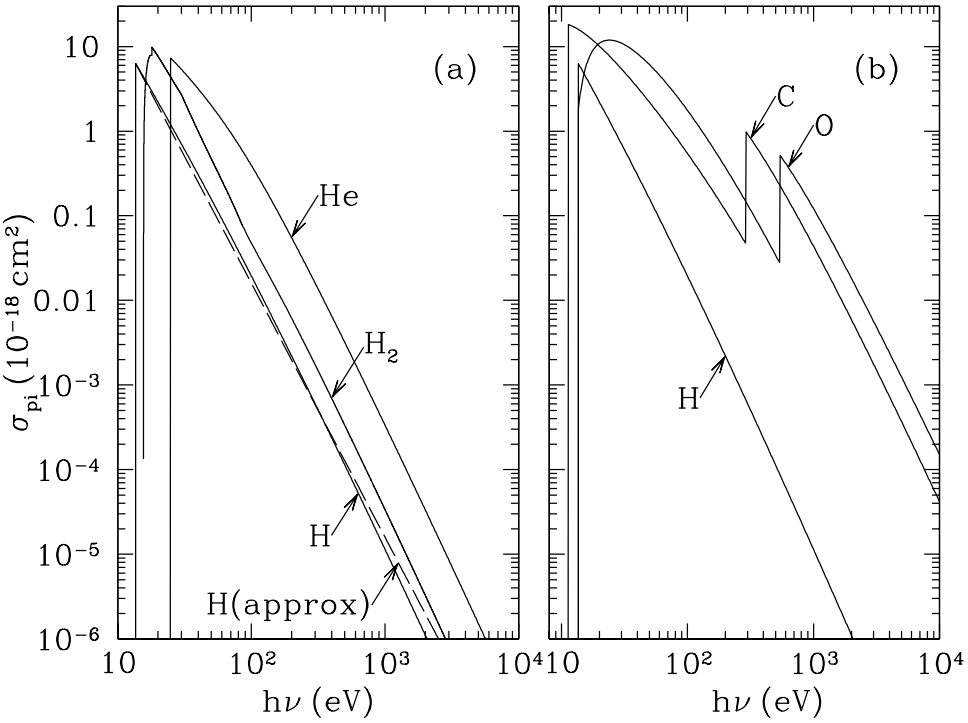

Figure 1: Figure 13.1 from Draine.

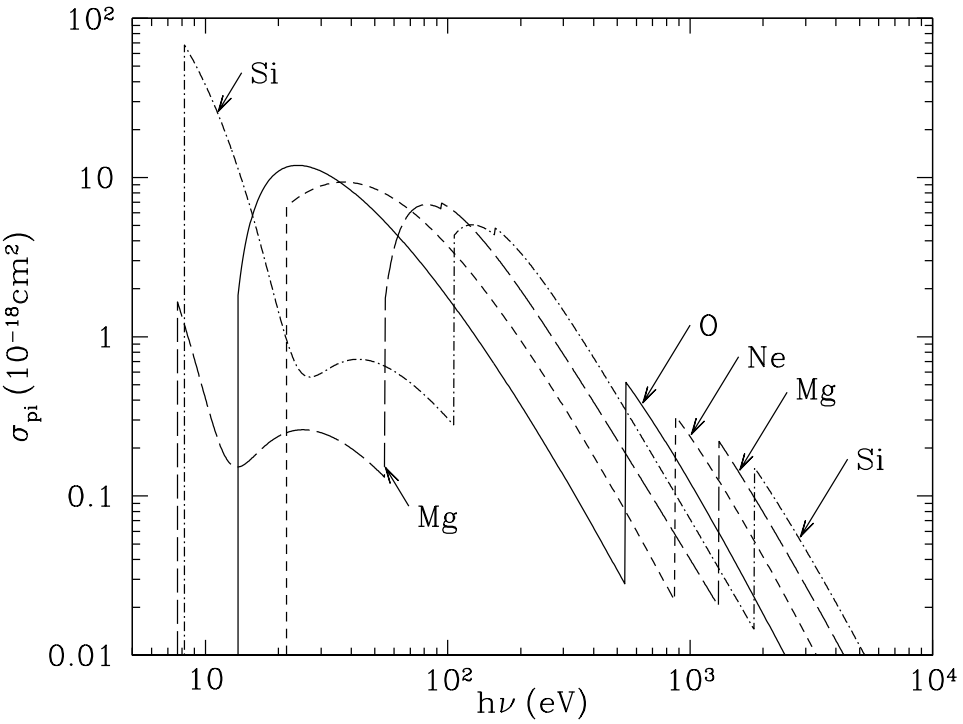

Figure 2: Figure 13.2 from Draine.

1 Oxygen: An Exemplar

Consider O I, for instance. A photon with energy greater than the ionization potential of 13.618 eV will result in the valence electron, $2s^2 2p^4\ ^3$P ejected to the continuum. However, the run of photo-ionization cross-section of O I with energy shows considerable complexity (see Figure 3) that is conspicuously absent in the run of the cross-section of hydrogen.The Grotrian diagram of O^+ (Figure 5) helps us understand the new pathways that are available to the incident ionizing photon.

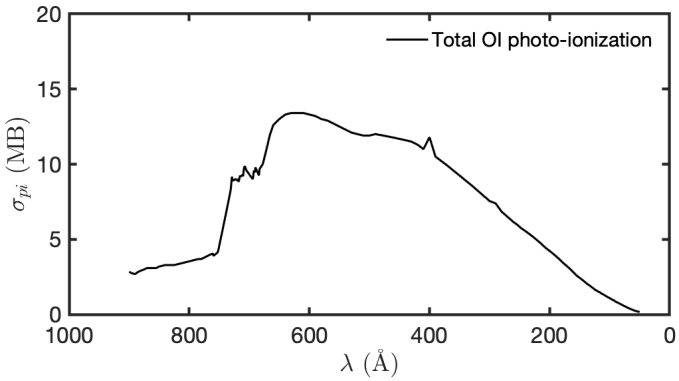

Figure 3: The total photo-ionization cross-section for O^0 to O^+ as a function of wavelength. Here, MB stands for Mega-barn which is 10^{-18} cm^2. Drawn from data provided by Angel & Samson (1988).

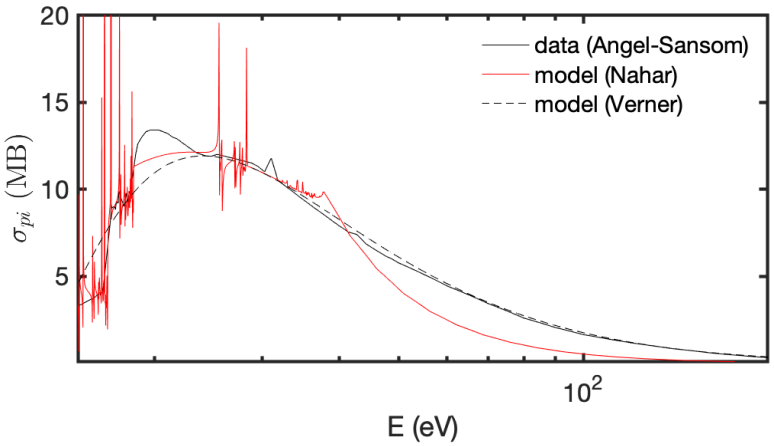

Figure 4: Comparison of experimental data (Angel & Samson 1988) to computer model calculations (Nahar 1999).

The ground state of the O^+ ion is $2s^2 2p^3\ ^4$S. Let us increase the energy of the incident

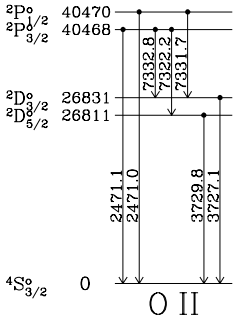

Figure 5: Grotrian diagram of O II showing first few levels.

photon. As can be seen from Figure 5 the ground state is $2s^2 2p^3\ ^4$S and the first two excited states are $2s^2 sp^3\ ^2$D (3.3 eV) (and $2s^2 2p^3\ ^2$P (5.02 eV). Thus a photon with energy $E = 13.6 + 3.3 = 16.9$ eV can both photo-ionized an O^0 atom and leave the O^+ ion in the first excited state, ^{2}D state. Shortly thereafter the O^+ ion relaxes by emitting 3628 Åphoton. Likewise, for $E = 13.6 + 5.0 = 18.6$ eV photon the ending state is a free electron and O^+ in the ^{2}P state. With this model in mind the run of the photo-ionization cross-section with E is decomposed to reflect the different pathways.

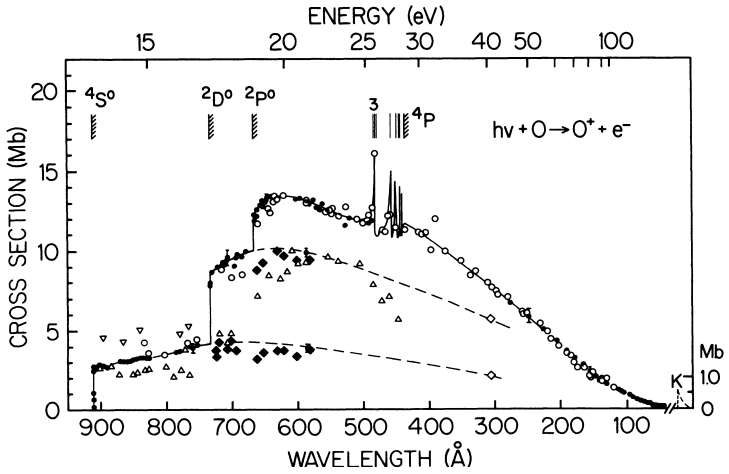

Figure 6: (Top): (Bottom): Experimental data with decomposition shown; from Angel & Samson (1988).

For pathways involving ionization and excitation it is more convenient to plot the Grotrian diagram with the zero point set by the ground state of the initial atom (ion), in

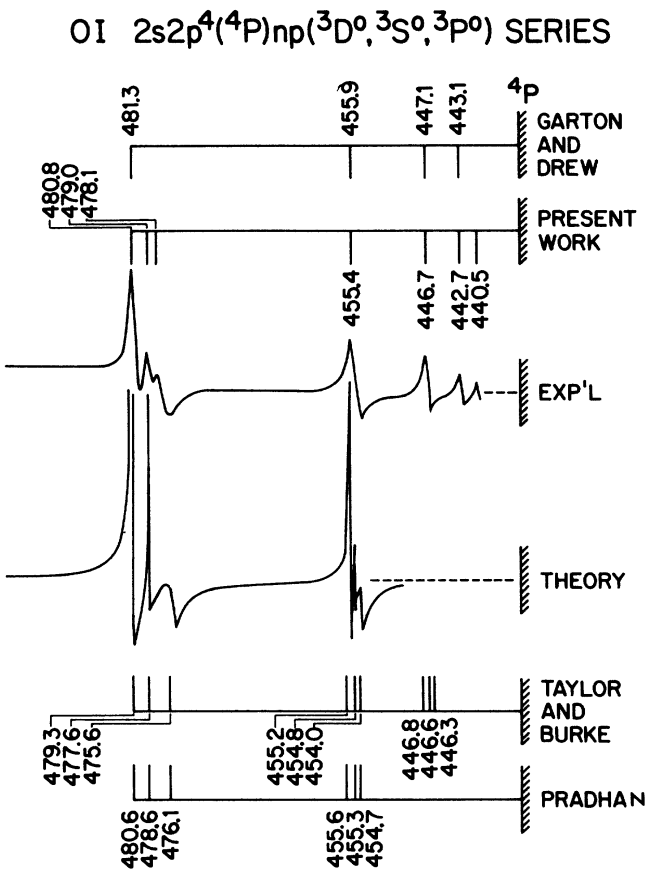

FIG. 4. Autoionizing resonances leading to the ^4P threshold; upper curve, the rate meter signal from the present experiment; lower curve, the theoretical predictions of Pradhan (Ref. 10). The upper wavelength assignments are those derived from the present work and the photographic measurements of Garton and Drew (Ref. 40), the lower are those reported by Pradhan (Ref. 10), and Taylor and Burke (Ref. 8).

Figure 7:

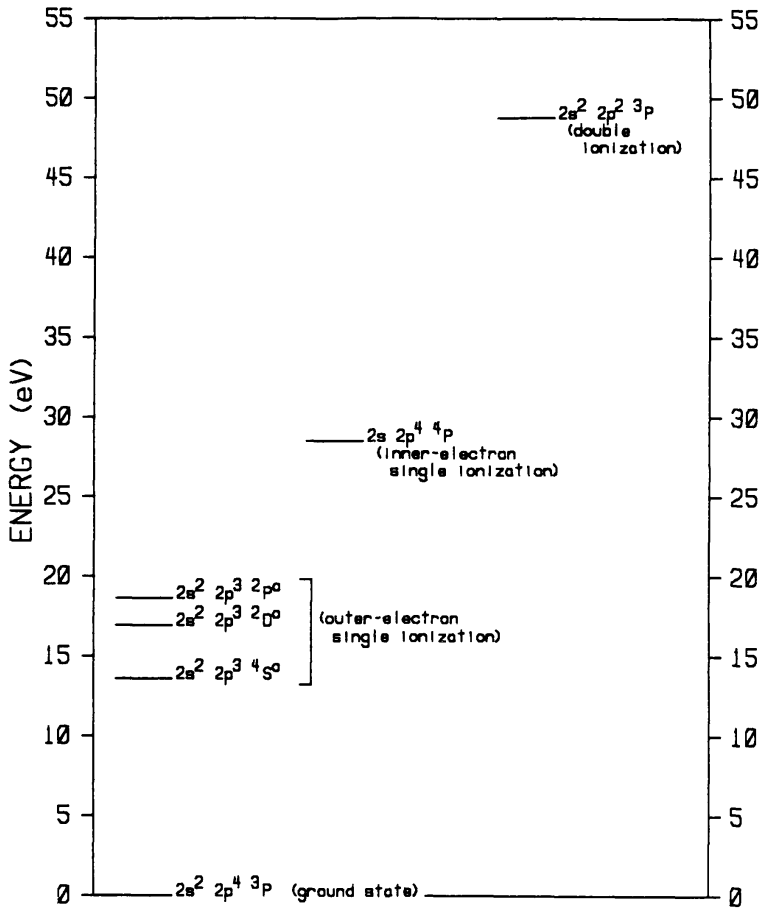

Figure 8: Grotrian diagram for O I (from Laher & Gilmore 1988).

this case, O^0. This figure also shows new pathways: (1) the inner electron is ionized which the leaves O^+ in the $2s2p^4\,{}^4P$ state and (2) the two outer electrons are ionized leaving O^+ in the $2s^2p^2\,{}^3P$ state.

1.1 Fluorescence

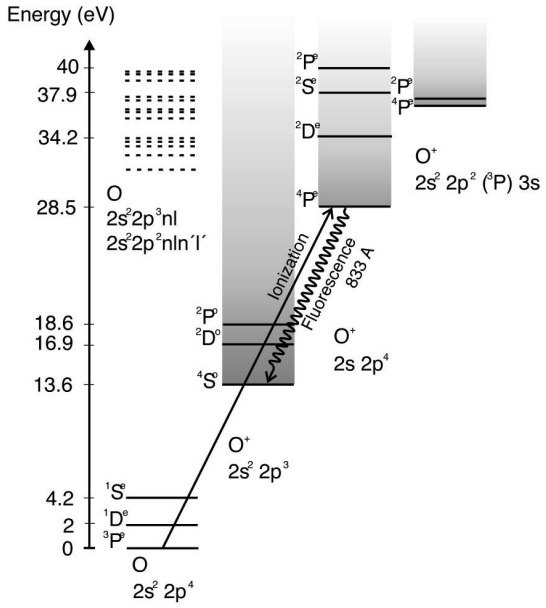

TABLE I. Photoionization processes in atomic oxygen investigated in the present study. The synchrotron radiation energy $h\nu_{SR}$ necessary to reach the excited singly ionized state is given in eV, and the fluorescence wavelength λ (in units of Å) for the transition into the final ionic state [12] are included for completeness.

Ground state	Excited ionic state Threshold energy (eV)	Final ionic state Fluorescence wavelength (Å)
	$O^+(2s2p^4\ {}^4P^e)$	$O^+(2s^22p^3\ {}^4S^o)$
	$h\nu_{SR} \geqslant 28.5$ eV	λ = 833 Å
	$O^+(2s2p^4\ {}^2D^e)$	$O^+(2s^22p^3\ {}^2D^o, {}^2P^o)$
	$h\nu_{SR} \geqslant 34.2$ eV	λ = 719 Å,797 Å
	$O^+(2s2p^4\ {}^2S^e)$	$O^+(2s^22p^3\ {}^2P^o)$
$O(2s^22p^4\ {}^3P^e)$	$h\nu_{SR} \geqslant 37.9$ eV	λ = 644 Å
	$O^+(2s2p^4\ {}^2P^e)$	$O^+(2s^22p^3\ {}^2D^o, {}^2P^o)$
	$h\nu_{SR} \geqslant 40.0$ eV	λ = 538 Å,581 Å
	$O^+(2s^22p^2({}^3P)3s\ {}^4P^e)$	$O^+(2s^22p^3\ {}^4S^o)$
	$h\nu_{SR} \geqslant 36.6$ eV	λ = 539 Å
	$O^+(2s^22p^2({}^3P)3s\ {}^2P^e)$	$O^+(2s^22p^3\ {}^2D^o, {}^2P^o)$
	$h\nu_{SR} \geqslant 37.1$ eV	λ = 617 Å,673 Å

Figure 9: Grotrian diagram for ground and excited states of O^+. From Wilhelmi et al. 1999. The accompanying table is also from the same reference.

1.2 Multiple Electrons

Another question you may have in mind is whether a photon can eject more than one photo-electron. As can be seen from the Table below the cross-section for a single photon to eject multiple electrons is quite small.

TABLE II. Absolute photoionization cross section for single, double, and triple photoionization from 44 to 254 Å.

$h\nu$ (eV)	λ (Å)	O^+ (Mb)	O^{2+} (10^{-2} Mb)	O^{3+} (10^{-3} Mb)	σ_{tot} (Mb)
48.736	254.402	6.00	0.0		6.00
50	248.0	5.75	2.0		5.77
60	206.6	4.25	18.7		4.44
70	177.1	3.20	22.5		3.43
80	155.0	2.37	23.0		2.60
90	137.8	1.84	22.1		2.06
100	124.0	1.44	20.5		1.65
110	112.7	1.20	18.5	0.28	1.39
120	103.3	1.01	16.4	1.01	1.17
130	95.4	0.86	14.2	1.65	1.00
140	88.6	0.72	12.1	2.02	0.84
150	82.7	0.62	10.3	2.20	0.73
160	77.5	0.52	8.4	2.12	0.61
170	72.9	0.45	6.9	1.95	0.52
180	68.9	0.39	5.8	1.75	0.45
190	65.3	0.33	4.8	1.51	0.38
200	62.0	0.286	3.9	1.28	0.33
210	59.0	0.250	3.2	1.07	0.28
220	56.4	0.220	2.55	0.87	0.25
230	53.9	0.197	2.05	0.69	0.22
240	51.7	0.180	1.75	0.54	0.20
250	49.6	0.168	1.50	0.44	0.18
260	47.7	0.161	1.30	0.37	0.17
270	45.9	0.154	1.20	0.32	0.17
280	44.3	0.150	1.05	0.27	0.16

1.3 High Energy Photo-absorption

The is summarized in Figure 10

2 Recombination: Radiative & Dielectronic

Again we start with hydrogen. There is only one path for recombination, namely radiative recombination (RR). This is a very slow process. For multiple electron systems there are new pathway.

In radiative recombination an electron from the continuum, upon recombination, emits a photon with energy equal to the sum of the kinetic energy of the electron and the potential energy of the line to which it recombines. In di-electronic recombination the same energy

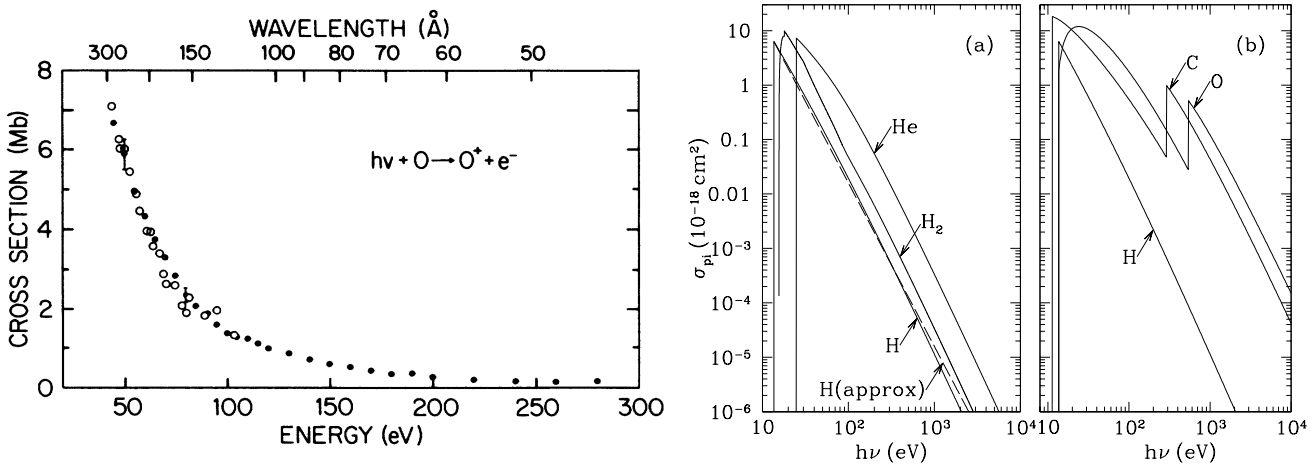

Figure 10: The high-energy cross section for single ionization of oxygen. (Right) From Angel & Samson (1988). (Left) From Draine (2011) emphasizing the K-shell absorption.

is excite another electron of the recombined atom/ion. Thus, the recombined atom/ion is in a doubly excited state. There are two outcomes. One electron is ejected ("auto-ionization") or the system could relax by emitting one or two photons and recombination is now complete ("di-electronic" recombination, DR). Clearly, DR process is resonant (i.e. the energy of the electron must equal the exact sums of two levels).

The classical DR process relies on exciting the valence electron of the recombined atom/ion to the first resonance level. Typically the first available resonance line is a good fraction of the ionization potential. Thus, DR, in most cases, becomes important at high temperatures.

There are two exceptions to the rule that DR dominates at high temperature (cf. the HIM). At low temperatures, following recombination one electron could be in a high Rydberg state and the other in an excited fine structure line of the ground term. Clearly, the recombining electron does not need to have large energy in this case. Examples include C II $\rightarrow$ C I, Si II $\rightarrow$ Si I and O III $\rightarrow$ O II (Bryans et al. 2009).

The other exception is the recombination of C III and Mg II in H II regions.

The total recombination coefficient is plotted in Figure 13.

References

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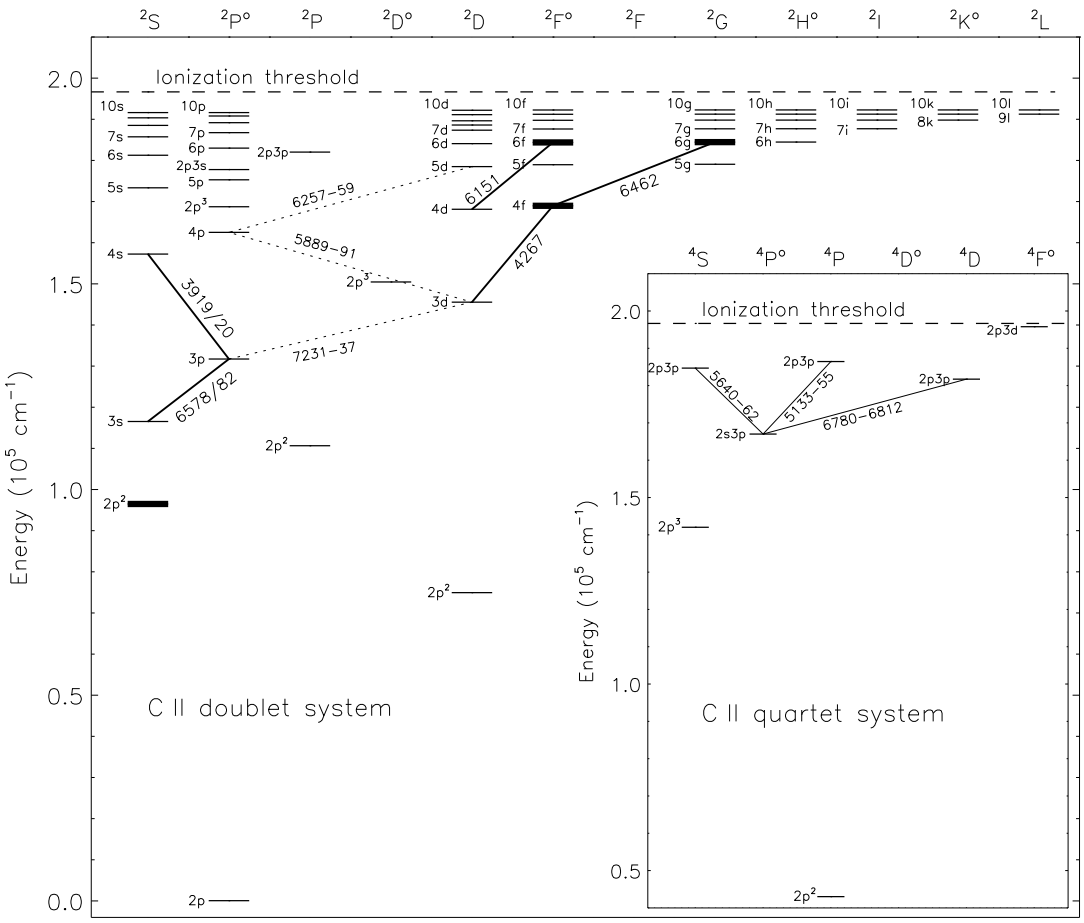

Figure 11: M. F. Nieva and N. Przybilla, 2008, A & A

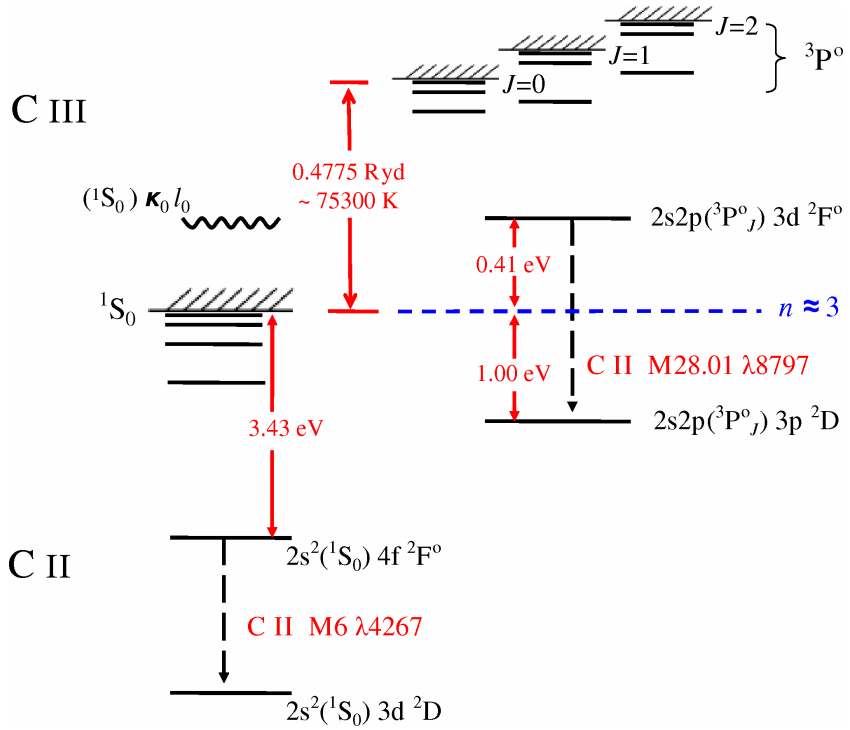

Figure 10. Schematic figure showing the dielectronic recombination of C II through the autoionizing state between the ionization thresholds $2s^2\,{}^1S_0$ and $2s2p\,{}^3P^o_J$ of C III. The electrons captured to the $2s2p({}^3P^o_J)3d\,{}^2F^o$ autoionizing state either go back to a true continuum state $2s^2({}^1S_0)\kappa_0 l_0$ through autoionization, or decay to the $2s2p({}^3P^o_J)3p\,{}^2D$ bound state through the C II M28.01 λ8797 transition. Also shown is the C II M6 λ4267 radiative recombination transition between the $4f\,{}^2F^o$ and the $3d\,{}^2D$ bound states.

Figure 12: X. Fang and X. -W Liu, MNRAS (2011)

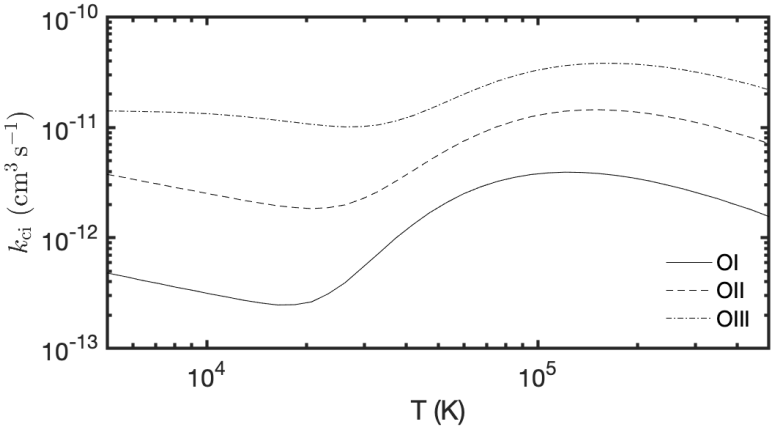

Figure 13: (Model) Recombination rate coefficient for oxygen (from Nahar 1999). At low temperatures the recombination coefficient declines with increasing temperature. The increase in the coefficient at mid temperatures (10^5 K) is due to dielectronic recombination.