

PHOTO-IONIZATION CROSS-SECTIONS FOR IONS OF CARBON, NITROGEN, OXYGEN, AND NEON

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Received February 14, 1968

ABSTRACT

Photo-ionization cross-sections are presented for C III, C IV, C V, N III, N IV, N V, O III, O IV, O V, Ne II, Ne III, Ne IV, and Ne V, as calculated by the screening theory, the quantum-defect method (where possible), and the hydrogenic approximation. These ions contribute to the opacity in the atmospheres of the central stars of planetary nebulae.

In this paper, results are presented for calculations of photo-ionization cross-sections for the following ions: C III, C IV, N III, N IV, N V, O III, O IV, O V, Ne II, Ne III, Ne IV, and Ne V. The wavelength range covered is $39.1 \leq \lambda \leq 867.9 \text{ \AA}$, which corresponds to an energy range of $1.05 \leq h\nu \leq 23.3 \text{ Ryd}$.

These ions are important sources of opacity on the O'Dell (1963) and Harman-Seaton (1964) sequences of central stars of planetary nebulae, as pointed out by Böhm and Deinzer (1965). Böhm and Deinzer have accounted for the opacity from the ground states of the above-named ions, using the hydrogenic approximation. The present calculation extends the result to excited states which can also contribute to the opacity (see Table 1) and uses the screening theory (ST) developed by Layzer (1959) and the quantum-defect method (QDM) of Burgess and Seaton (1960), as well as the hydrogenic approximation (HA). The results thus allow a direct check upon the consistency of the two more physical theories, and an estimate of the error made with the HA.

The QDM was used only in C IV, N III, N V, and O V, because the irregularities that appeared in the quantum-defect series for the other elements made its application doubtful. Also in many cases, for example, ions of neon, lack of spectroscopic data made the construction of the series impossible. The energy levels were obtained from Moore's tables (1949), except for the case of N V, where we used more recent data by Tilford (1963). Extensive use of the tables published by Peach (1967) was made to obtain the QDM radial integrals. The interpolation in those tables was done using a parabolic formula. The other parameters used in the QDM are listed in Table 2.

The calculation of the cross-sections using ST was performed introducing the simple screening constants obtained by Layzer (1959). No account is taken of the irregular solution for the radial wave functions when we use ST. We assume, in all cases, the dipole approximation, non-relativistic treatment of the particles, *LS* coupling, and orthogonality between the final ion and the core of the atom.

In those cases where both theories could be used, there is remarkable agreement between the results obtained using QDM and ST. The values given by the ST are generally a little bit larger than the ones obtained with the QDM. The good agreement lends confidence to the accuracy of the result. The closeness of the ST result with those of the QDM is a consequence of dealing with very high ionized atoms, since in that case the screening theory is supposed to be a fairly good approximation. We also note that, in general, the values given by the HA are smaller than the ones obtained with the other two methods. Generally, the disagreement with the HA is worse for configurations which are not even approximately hydrogenic and for which the HA could not really be expect-

TABLE 1
BOUND STATES FOR WHICH PHOTO-IONIZATION CROSS-SECTIONS
HAVE BEEN CALCULATED

Ion	Configuration	χ_{exe} (cm ⁻¹)	$\lambda_{\text{threshold}}$ (Å)	Level No.
Ne V . . .	$2s^2 2p^2 \ ^3P$	755.77	98.2436	1
Ne V . . .	$2s^2 2p^2 \ ^1D$	30294	101.1797	2
Ne V . . .	$2s^2 2p^2 \ ^1S$	63900	104.7412	3
Ne V . . .	$2s^2 2p^3 \ ^5S$	88842	107.5509	4
O V . . .	$2s^2 \ ^1S$	0.0	108.8492	5
O V . . .	$2s(^2S)2p \ ^3P$	82412.822	119.5758	6
N V . . .	$2s^2 \ ^1S$	0.0	126.6571	7
Ne IV . . .	$2s^2 2p^3 \ ^4S$	0.0	127.7517	8
O V . . .	$2s(^2S)2p \ ^1P$	158798	131.5955	9
Ne IV . . .	$2s^2 2p^3 \ ^2D$	40968	134.8072	10
Ne IV . . .	$2s^2 2p^3 \ ^2P$	62157	138.7711	11
N V . . .	$2p \ ^2P$	80636.766	141.0643	12
O IV . . .	$2s^2(^1S)2p \ ^2P$	257.666	160.0220	13
N IV . . .	$1s^2 2s^2 \ ^1S$	0.0	160.0381	14
Ne IV . . .	$2s^2 2p^4 \ ^4P$	184222.166	167.0715	15
N IV . . .	$1s^2 2s^2 2p \ ^3P^o$	67272.68	179.3470	16
O IV . . .	$2s^2 2p^4 \ ^4P$	71378.75	180.8260	17
C IV . . .	$2s^2 \ ^1S$	0.0	192.2419	18
Ne III . . .	$2s^2 2p^4 \ ^3P$	317.3	194.6166	19
O IV . . .	$2s^2 2p^2 \ ^2D$	126941.9	201.0233	20
N IV . . .	$1s^2 2s^2 2p \ ^1P^o$	130695	202.3652	21
Ne III . . .	$2s^2 2p^4 \ ^1D$	25840.8	204.7891	22
Ne III . . .	$2s^2 2p^4 \ ^1S$	55747	218.1496	23
C IV . . .	$2p \ ^2P$	64555.6	219.4801	24
O III . . .	$2s^2 2p^2 \ ^3P$	208.244	225.9382	25
O III . . .	$2s^2 2p^2 \ ^1D$	20271	236.6662	26
O III . . .	$2s^2 2p^2 \ ^1S$	43183.5	250.2355	27
C III . . .	$2s^2 \ ^1S$	0.0	258.9238	28
N III . . .	$2p \ ^2P$	116.333	261.4316	29
O III . . .	$2s^2 2p^3 \ ^5S$	60312.1	261.4413	30
C III . . .	$2s(^2S)2p \ ^3P$	52367	299.5385	31
Ne II . . .	$2s^2 2p^5 \ ^2P$	260.666	302.0332	32
N III . . .	$2s^2 2p^2 \ ^4P$	57282.616	307.3680	33
C III . . .	$2s(^2S)2p \ ^1P$	102351.4	352.2832	34
N III . . .	$2s^2 2p^2 \ ^2D$	101026.88	355.1153	35
C IV . . .	$3s^2 \ ^1S$	302847.9	460.1299	36
Ne II . . .	$2s^2 2p^6 \ ^2S$	217050	874.8906	37

TABLE 2
VALUES OF THE QUANTUM DEFECTS USED ($\mu_l = A_l + B_l \epsilon$)

Element	$l=0$	$l=1$	$l=2$	Remarks
N III {A B	+0.514 - .0706	+0.266 - .327	$+7.17 \times 10^{-2}$ -0.023	Series $2s^2(^1S)nl$
N V {A B	+ .128 - .026	+ .034 + .0057	$+2.36 \times 10^{-3}$ +0.0093	Series $(1s^2)nl$
O V {A B	+ .202 - .207	+ .112 + .046	+0.018 +0.109	Series $1s^2(^2S)nl$ singlet
O V {A B	+ .232 - .375	+ .105 - .272	+0.048 -0.100	Series $1s^2(^2S)nl$ triplet
C IV {A B	+ .154 -0.029	+ .038 +0.006	$+2.33 \times 10^{-3}$ +0.007	Series $(1s^2)nl$

TABLE 3
VALUES OF THE CROSS-SECTIONS IN MB (10^{-18} cm²)
(Level Number and Theory Used)

LAMBDA (Å)	1 ST	2 ST	3 ST	4 ST	5 ST	5 QD	6 ST	6 QD	7 ST	7 QD	8 ST	9 ST	9 QD	10 ST	11ST	12 ST	12 QD
141.1																5.9-1	5.9-1
138.5															4.0+0	5.6-1	6.8-1
136.0															3.9+0	5.3-1	6.5-1
133.6														4.1+0	3.8+0	5.0-1	6.1-1
131.3												6.9-1	6.4-1	3.9+0	3.7+0	4.8-1	5.8-1
129.1												6.5-1	7.1-1	3.8+0	3.6+0	4.5-1	5.5-1
126.9											6.2+0	6.2-1	6.8-1	3.8+0	3.5+0	4.3-1	5.2-1
124.8									5.7-1	6.4-1	4.1+0	5.9-1	6.5-1	3.7+0	3.4+0	4.1-1	4.9-1
119.0						7.9-1	7.5-1	5.2-1	4.0-1	3.8+0	3.8+0	5.1-1	5.6-1	3.4+0	3.2+0	3.5-1	4.2-1
117.1						7.6-1	8.9-1	5.0-1	3.9-1	3.7+0	3.7+0	6.9-1	5.3-1	3.3+0	3.1+0	3.4-1	4.0-1
115.4						7.2-1	8.6-1	4.9-1	3.8-1	3.6+0	3.6+0	4.7-1	5.1-1	3.2+0	3.0+0	3.2-1	3.8-1
113.6						6.9-1	8.3-1	4.7-1	3.7-1	3.5+0	3.5+0	4.5-1	4.9-1	3.1+0	3.0+0	3.0-1	3.6-1
111.9						6.6-1	7.9-1	4.6-1	3.6-1	3.5+0	3.5+0	4.3-1	4.6-1	3.1+0	2.9+0	2.9-1	3.5-1
108.7					7.6-1	7.3-1	7.4-1	4.4-1	3.4-1	3.3+0	3.3+0	3.9-1	4.3-1	2.9+0	2.7+0	2.6-1	3.2-1
107.2				2.5+0	7.5-1	7.2-1	7.1-1	4.3-1	3.3-1	3.2+0	3.2+0	3.7-1	4.1-1	2.8+0	2.7+0	2.5-1	3.0-1
104.3			1.8+0	2.4+0	7.4-1	6.9-1	6.6-1	4.0-1	3.2-1	3.1+0	3.1+0	3.5-1	3.8-1	2.7+0	2.5+0	2.3-1	2.8-1
100.1		1.8+0	1.7+0	2.3+0	7.1-1	6.5-1	6.0-1	3.7-1	2.9-1	2.8+0	2.8+0	3.0-1	3.3-1	2.5+0	2.4+0	2.1-1	2.4-1
97.6	1.9+0	1.7+0	1.6+0	2.2+0	6.9-1	6.2-1	5.6-1	3.5-1	2.8-1	2.7+0	2.7+0	2.8-1	3.1-1	2.4+0	2.2+0	1.9-1	2.2-1
80.9	1.2+0	1.1+0	1.0+0	1.5+0	5.6-1	4.6-1	3.6-1	3.6-1	1.9-1	1.8+0	1.8+0	1.5-1	1.7-1	1.6+0	1.5+0	1.0-1	1.2-1
39.1	1.5-1	1.4-1	1.3-1	2.5-1	1.5-1	1.1-1	8.6-2	4.6-2	4.2-2	2.5-1	2.5-1	1.4-2	1.7-2	2.3-1	2.2-1	9.2-3	1.1-2

68.5 2.3-1 4.6-2 4.6-1 2.2-2 1.9+0 1.3-1 1.1-2 9.8-2 2.3-2 2.3-2 1.7+0

TABLE 3—Continued

LAMBDA (Å)	13 ST	14 ST	15 ST	16 ST	17 ST	18 ST	18 QD	19 ST	20 ST	21 ST	22 ST	23 ST	24 ST	24 QD	25 ST	26 ST	27 ST
246.3																	4.9+0
231.3																5.0+0	4.4+0
224.5												5.3+0			5.3+0	4.8+0	4.2+0
218.0												5.7+0	9.3-1	9.3-1	5.0+0	4.5+0	4.0+0
211.9												5.6+0	8.5-1	9.9-1	4.8+0	4.3+0	3.8+0
206.2												5.6+0	7.8-1	9.1-1	4.6+0	4.1+0	3.6+0
200.7									2.4+0	1.1+0	5.9+0	5.6+0	7.2-1	8.4-1	4.4+0	3.9+0	3.4+0
190.6						8.7-1	6.4-1	6.2+0	2.2+0	9.5-1	5.8+0	5.5+0	6.2-1	7.1-1	3.9+0	3.5+0	3.1+0
177.3				1.3+0	2.5+0	7.7-1	5.7-1	6.0+0	1.9+0	7.7-1	5.7+0	5.3+0	4.9-1	5.6-1	3.4+0	3.0+0	2.7+0
165.7			3.9+0	1.0+0	2.2+0	6.8-1	5.0-1	5.8+0	1.7+0	6.3-1	5.5+0	5.1+0	4.0-1	4.5-1	2.9+0	2.6+0	2.3+0
158.8	1.5+0	9.1-1	3.8+0	9.4-1	2.0+0	6.3-1	4.7-1	5.6+0	1.5+0	5.5-1	5.3+0	4.9+0	3.5-1	3.9-1	2.7+0	2.4+0	2.1+0
120.9	6.8-1	7.7-1	2.9+0	4.1-1	1.1+0	3.7-1	2.8-1	4.2+0	8.8-1	2.4-1	3.9+0	3.6+0	1.5-1	1.6-1	1.4+0	1.2+0	1.1+0
100.1	3.9-1	6.3-1	2.3+0	2.2-1	7.2-1	2.4-1	1.9-1	3.2+0	5.6-1	1.3-1	3.0+0	2.7+0	8.0-2	9.0-2	8.3-1	7.4-1	6.6-1
80.9	1.9-1	4.6-1	1.6+0	1.1-1	4.1-1	1.5-1	1.3-1	2.1+0	3.2-1	6.5-2	2.0+0	1.8+0	3.9-2	4.5-2	4.4-1	4.0-1	3.5-1
68.5	1.1-1	3.4-1	1.2+0	6.4-2	2.6-1	1.0-1	8.9-2	1.5+0	2.0-1	3.7-2	1.4+0	1.3+0	2.2-2	2.6-2	2.6-1	2.4-1	2.1-1
LAMBDA (Å)	28 ST	29 ST	29 QD	30 ST	31 ST	32 ST	33 ST	34 ST	35 ST	36 ST	36 QD	37 ST					
867.9												1.7+0					
828.4												1.8+0					
792.4												1.9+0					
560.8												2.9+0					
461.4												3.5+0					
455.6										1.4+0	1.0+0	3.5+0					
428.8										1.3+0	9.4-1	3.7+0					
400.6										1.2+0	8.3-1	3.9+0					
364.5										9.8-1	7.0-1	4.1+0					
347.8								2.0+0	3.9+0	8.9-1	6.5-1	4.2+0					
305.8							4.4+0	1.4+0	3.3+0	7.0-1	5.1-1	4.5+0					
294.0							4.2+0	1.3+0	3.1+0	6.5-1	4.8-1	4.6+0					
254.5	9.1-1	2.7+0	2.0+0	5.8+0	2.4+0	5.5+0	3.3+0	8.4-1	2.5+0	4.8-1	3.6-1	4.8+0					
246.3	9.4-1	2.5+0	1.9+0	5.6+0	1.5+0	6.7+0	3.2+0	7.6-1	2.3+0	4.5-1	3.4-1	4.8+0					
238.6	9.6-1	2.3+0	1.8+0	5.5+0	1.3+0	6.8+0	3.0+0	6.9-1	2.2+0	4.2-1	3.2-1	4.8+0					
206.2	1.0+0	1.5+0	1.3+0	4.6+0	8.7-1	7.2+0	2.3+0	4.4-1	1.7+0	3.1-1	2.4-1	4.8+0					
186.0	9.9-1	1.1+0	1.0+0	4.0+0	6.3-1	7.2+0	1.8+0	3.2-1	1.4+0	2.5-1	2.0-1	4.7+0					
152.4	8.6-1	6.4-1	6.9-1	2.9+0	3.3-1	6.6+0	1.2+0	1.7-1	8.8-1	1.6-1	1.3-1	4.4+0					
100.1	4.9-1	1.7-1	3.0-1	1.2+0	8.3-2	4.1+0	3.9-1	4.2-2	3.0-1	6.3-2	5.7-2	3.0+0					

ed to be valid. It is interesting that for Ne II $2s^2 2p^5 \ ^2P$, Ne II $2s 2p^6 \ ^2S$, C IV $2p \ ^2P$, C IV $2s \ ^2S$, N III $2s 2p^2 \ ^2D$, and N V $2s \ ^2S$, the cross-sections show small discrepancies near threshold. In some of these cases, the cross-sections at first increase and then decrease, in contrast to the monotonic decrease given by the HA. Presumably these trends are real and are merely a result of the ST and QDM giving more details of the behavior of the cross-sections while the HA provides rather rough estimates.

Work is in progress to incorporate these results into calculation of model atmospheres of the nuclei of planetary nebulae.

This work has been supported by National Science Foundation grant GP-7761.

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1968ApJ...153..981H