Atomic Database for C I from C II

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1 Introduction

Carbon is the main constituent of the graphite tiles which cover the inner side of the vacuum chamber of the latest tokamaks (JET, TFTR, JET-60). Carbon is also one of the most abundant elements of the Universe. The tokamak spectra are very rich in C lines emitted in the outer region of the plasma, the coolest part, where C is not completely ionized and can still emit a line spectrum. The recombination rates will play an important role in the plasma cooling when more ionized species recombine progressively.

The dielectronic recombination (DR) process for C (C I from C II) can be schematically represented by $1s^22s^22p + e \Rightarrow 1s^22s2p^2nl,\ 1s^22s2p^3(LS),\ 1s^22p^3nl,\ 1s^22p^4$

$$\Downarrow \qquad \Downarrow$$

$$1s^22s^22p, 1s^22s2p^2 + e \ or\ 1s^22s^22p^2, 1s^22s^22pnl, 1s^22s2p^3(L'S') + h\nu\,, \tag{1}$$

where LS= ^3S, ^1D, ^1P for autoionizing states and $L'S'$=^5S, ^3D, ^3P for bound states. An intensity factor Q_d for transitions from autoionizing levels γ=$1s^22s2p^2nl$, $1s^22s2p^3(LS)$, $1s^22p^3nl$, $1s^22p^4$ to excited states γ'= $1s^22s^22p^2$, $1s^22s^22pnl$, $1s^22s2p^3(L'S')$ can be defined as follows:

$$Q_d(\gamma,\gamma'|\alpha_0) = g_\gamma A_r(\gamma,\gamma')\frac{A_a(\gamma,\alpha_0)}{A_r(\gamma)+A_a(\gamma)}, A_r(\gamma) = \sum_{\gamma''} A_r(\gamma,\gamma''),\ A_a(\gamma) = \sum_{\alpha'} A_a(\gamma,\alpha')\,, \tag{2}$$

where $A_r(\gamma,\gamma')$ are radiative transition probabilities and $A_a(\gamma,\alpha')$ is the autoionization rate, with α'=$1s^22s^22p$, $1s^22s2p^2$ and α_0= $1s^22s^22p$.

We used the Cowan [1] and $SUPERSTRUCTURE$ codes taking into account 28 even and 29 odd parity configurations $1s^22l_12l_22l_3nl$ with up to n=6 and 0≤ l ≤(n-1). The contributions of the configurations with 6≤ n ≤500 are taken into account in the calculation of all $1s^22l_12l_22l_3nl[LSJ]$ states up to n=6. In the present paper we can present only a small amount of our numerical data due to the limited space.

2 Energy Levels, Radiative Transition Probabilities

We carried out detailed calculations of radiative transition probabilities and autoionization rates for the intermediate states $1s^22s^22pnl$, $1s^22s2p^3$, $1s^22p^4$, $1s^22s2p^2nl$ and $1s^22p^3nl$ with n=2 - 6 . The atomic energy levels, radiative transition probabilities and autoionization rates were obtained by using the atomic structure code of Cowan [1]. Table 1 lists energies calculated by the *Cowan* (a) and $SUPERSTRUCTURE$ (b) codes, together with theoretical data obtained by Nahar and Pradhan (c) [2] and recommended data (d) by Wiese et al. [3] for C I with the $1s^22s^22p^2$, $1s^22s2p^3$, $1s^22s^22pnl$ intermediate states. The differences in the theoretical data (a) and (b) can be explained by different refinements of the Hartree-Fock approximation. The *Cowan* code allows the use of scaled factors for radial integrals. We used a scaled factor equal to 0.85. The $SUPERSTRUCTURE$ code is based on a scaled Thomas-Fermi-Dirac-Amadi potential. The scaling parameter is different for each angular momentum l. These parameters are iterated to give the minimum energy of a term or a group of terms. It should be noted that both methods did not take into account correlation effects properly which explains the disagreement of these data (columns a and b in Table 1) with the recommended data (column c) for some states.

3 Total Dielectronic Recombination Rate Coefficients

The total dielectronic recombination rate coefficient is obtained by the sum over all the levels,

$$\alpha_d^t(\alpha_0) = 3.3 \times 10^{-24} \left(\frac{I_H}{T_e}\right)^{3/2} \sum_{\gamma,\gamma'} e^{-\frac{E_S}{T_e}} Q_d(\gamma,\gamma'|\alpha_0)/g(\alpha_0)\,. \tag{3}$$

The sum over γ means sum over all autoionization levels. As we already mentioned before we calculated numerically the $Q_d(\gamma,\gamma'|\alpha_0)$ values with γ'=$1s^22s^22pnl$, $1s^22s2p^3$ (^5S, ^3D, ^3P) and γ=$1s^22s2p^3$ (^3S, ^1D, ^1P), $1s^22p^4$, $1s^22s2p^2nl$, $1s^22p^3nl$ up to n=6. We take into account the states with $n \geq$6 by scaling Q_d. It was shown in Ref.[4] that the largest contribution to Q_d for large n are due to the $2s$-$2p$ transitions. In our case it is transitions as $2s^22pnl[LS]$-$2s2p^2(LS)nl[L'S']$. Radiative transition probabilities for these transitions are almost constant for large n and non-radiative transition probabilities (autoionizing rates) are proportional to $\frac{1}{n^3}$:

$$A_r(2s^22pnl[LS],\ 2s2p^2(L_{12}S_{12})nl[L'S'J']) = A_r(2s^22pn_0l[LS],\ 2s2p^2(L_{12}S_{12})n_0l[L'S'J'])\,, \tag{4}$$

$$A_a(2s2p^2(L_{12}S_{12})nl[L'S'J']|\ 2s^22p\ ^2P) = \left(\frac{n_0}{n}\right)^3 A_a(2s2p^2(L_{12}S_{12})n_0l[L'S'J']|\ 2s^22p\ ^2P)\,. \tag{5}$$

Table 2 gives these data for n=4, 5, 6 with l=s, p, d, f, g and all kinds of $L'S'J'$. We chose for illustration the data with the largest values of Q_d. We can see from this Table that Eqs.(4,5) are correct for transitions with large values of A_r and A_a.

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Table 1: Energy ($10^3 cm^{-1}$) and sum of weighted radiative transition probabilities ($\sum(gA_r)$ in sec^{-1}) of carbon (C I) for $1s^2 2s2l_1 2l_2 (L_{12}S_{12})nl[LSJ]$ states. Comparison of different methods and recommended data from Ref.[3]: a-Cowan code, b-SUPERSTRUCTURE code, c-Ref.[2], d -Ref.[3]

$2s2l_1nl_2$	$L_{12}S_{12}$	LS	J	E in $10^3 cm^{-1}$				$\sum(gA_r)$
				a	b	c	d	a
$2s^2 2p^2$	(^3P)	^3P	0	0.000	0.000	0.000	0.000	0.0000+00
$2s^2 2p^2$	(^1D)	^1D	2	10.651	13.398	10.502	10.194	0.0000+00
$2s^2 2p^2$	(^1S)	^1S	0	18.953	20.411	23.023	21.648	0.0000+00
$2s^2 2p3p$	(^2P)	^1P	1	66.496	66.608	69.661	68.858	0.2661+08
$2s^2 2p3p$	(^2P)	^3D	2	67.069	67.403	69.650	69.711	0.8172+08
$2s^2 2p3p$	(^2P)	^3S	1	67.776	68.401	71.855	70.744	0.5717+08
$2s^2 2p3p$	(^2P)	^3P	1	70.429	70.876	72.722	71.365	0.1337+09
$2s^2 2p3p$	(^2P)	^1D	2	71.863	73.077	74.248	72.611	0.2293+09
$2s^2 2p3p$	(^2P)	^1S	0	73.420	76.223	75.992	73.976	0.5352+08
$2s2p^3$	(^4S)	^5S	2	31.866	24.432	32.515	33.735	0.0000+00
$2s2p^3$	(^2D)	^3D	2	67.675	66.919	63.943	64.093	0.1710+10
$2s2p^3$	(^2P)	^3P	1	78.763	76.186	76.014	75.256	0.2419+10
$2s^2 2p3s$	(^2P)	^3P	1	58.402	58.689	60.585	60.353	0.9067+09
$2s^2 2p3s$	(^2P)	^1P	1	59.686	61.388	62.385	61.982	0.1219+10
$2s^2 2p3d$	(^2P)	^3P	1	75.570	80.375	80.996	79.319	0.4165+09
$2s^2 2p3d$	(^2P)	^1D	2	76.069	76.288	79.350	77.681	0.3626+09
$2s^2 2p3d$	(^2P)	^3D	2	76.606	77.050	80.119	78.307	0.1836+10
$2s^2 2p3d$	(^2P)	^1F	3	76.682	77.433	80.327	78.531	0.1767+10
$2s^2 2p3d$	(^2P)	^3F	3	76.429	76.739	79.965	78.216	0.3085+09
$2s^2 2p3d$	(^2P)	^1P	1	76.644	77.653	79.877	78.728	0.2985+09
$2s^2 2p4s$	(^2P)	^3P	0	76.383		79.680	78.105	1.453+08
$2s^2 2p4s$	(^2P)	^1P	1	76.932		79.877	78.338	7.806+08
$2s^2 2p4p$	(^2P)	^1D	2	80.914		83.168	81.770	1.012+08
$2s^2 2p4p$	(^2P)	^1S	0	82.434		83.794	82.252	5.231+07
$2s^2 2p4d$	(^2P)	^3D	1	82.147		85.681	83.830	6.559+08
$2s^2 2p4d$	(^2P)	^1F	3	82.241		85.780	83.949	1.989+09
$2s^2 2p5s$	(^2P)	^1P	1	82.443		85.661	83.882	3.972+08
$2s^2 2p5p$	(^2P)	^1D	2	84.186		87.062	85.400	4.708+07
$2s^2 2p5p$	(^2P)	^1S	0	84.613		87.325	85.626	1.312+07
$2s^2 2p5d$	(^2P)	^1F	3	84.868		88.300	86.450	7.044+08
$2s^2 2p5d$	(^2P)	^1P	1	84.860		88.358	86.491	1.335+08
$2s^2 2p6s$	(^2P)	^1P	1	84.940		88.253	86.414	2.338+08
$2s^2 2p6p$	(^2P)	^3P	0	85.625		88.877	87.077	4.477+06
$2s^2 2p6d$	(^2P)	^1D	2	86.127		89.489	87.632	1.786+08
$2s^2 2p6d$	(^2P)	^3F	2	86.160		89.599	87.706	2.013+08

Table 2: Energy excitation (E_S in eV), weighted radiative transition probabilities ((gA_r) in sec^{-1}), autoionization rate (A_a in sec^{-1}) and factor intensities (Q_d in sec^{-1}) for $2s^22pnl$-$2s2p^2(L_{12}S_{12})nl(L'S'J')$ transitions with n=4, 5, and 6.

	Upper level			A_a	$\sum(A_a)$	gA_r	$\sum(gA_r)$	Q_d	E_S
n	$L_{12}S_{12}$	$L'S'$	J'						
$2s^22pns$	$2s2p^2(L_{12}S_{12})ns(L'S'J')$								
4	(^1D)	^1D	2	7.702+13	1.502+14	2.712+09	1.027+09	8.914+07	7.948
5	(^1D)	^1D	2	3.574+13	7.562+13	3.327+09	1.338+09	1.104+08	8.599
6	(^1D)	^1D	2	2.426+13	5.127+13	2.577+09	1.398+09	1.293+08	8.897
$2s^22pnp$	$2s2p^2(L_{12}S_{12})np(L'S'J')$								
4	(^1D)	^1F	3	3.047+13	3.489+13	5.592+09	4.254+09	6.193+08	8.187
5	(^1D)	^1F	3	4.854+12	7.879+12	4.192+09	3.281+09	3.368+08	8.710
6	(^1D)	^1F	3	2.633+12	4.188+12	5.308+09	3.802+09	3.984+08	8.954
4	(^3P)	^3Pa	2	2.630+13	6.458+13	2.379+10	2.339+10	1.587+09	12.49
5	(^3P)	^3Pa	2	2.884+12	2.456+13	2.290+10	2.246+10	4.393+08	13.03
6	(^3P)	^3Pa	2	1.454+12	1.178+13	2.328+10	2.297+10	4.725+08	13.28
$2s^22pnd$	$2s2p^2(L_{12}S_{12})nd(L'S'J')$								
4	(^1S)	^3D	3	1.329+13	1.602+13	1.495+10	1.435+10	1.984+09	10.88
5	(^1S)	^3D	3	3.851+12	7.046+12	1.460+10	1.420+10	1.293+09	11.22
6	(^1S)	^3D	3	2.323+12	4.198+12	1.501+10	1.417+10	1.306+10	11.39
4	(^3P)	^3Fa	2	4.384+13	4.580+13	2.100+10	2.075+10	3.310+09	12.84
5	(^3P)	^3Fa	2	1.278+13	1.482+13	2.183+10	2.017+10	1.881+09	13.18
6	(^3P)	^3Fa	2	6.991+12	8.113+12	2.189+10	2.139+10	3.071+09	13.36
4	(^3P)	^1F	3	4.895+13	5.632+13	3.084+10	2.895+10	4.194+09	12.86
5	(^3P)	^1F	3	1.418+13	1.831+13	3.114+10	3.006+10	3.879+09	13.19
6	(^3P)	^1F	3	8.314+12	1.050+13	3.144+10	3.009+10	3.968+09	13.37
$2s^22pnf$	$2s2p^2(L_{12}S_{12})nf(L'S'J')$								
4	(^3P)	^1D	2	3.140+11	3.740+11	2.362+10	2.351+10	3.429+09	12.87
5	(^3P)	^1D	2	1.970+11	1.460+11	2.273+10	2.266+10	2.405+09	13.20
6	(^3P)	^1D	2	1.170+11	1.670+11	2.286+10	2.271+10	2.581+09	13.37
4	(^3P)	^3Ga	3	4.201+12	4.233+12	3.003+10	2.990+10	4.940+09	12.87
5	(^3P)	^3Ga	3	7.880+11	9.260+11	3.089+10	3.079+10	4.347+09	13.20
6	(^3P)	^3Ga	3	5.450+11	6.320+11	3.082+10	3.074+10	4.387+09	13.37
4	(^3P)	^1G	4	4.257+12	4.288+12	3.850+10	3.839+10	6.337+09	12.87
5	(^3P)	^1G	4	8.150+11	9.620+11	3.964+10	3.953+10	5.556+09	13.21
6	(^3P)	^1G	4	5.670+11	6.620+11	3.945+10	3.941+10	5.589+09	13.38
$2s^22png$	$2s2p^2(L_{12}S_{12})ng(L'S'J')$								
5	(^3P)	^1G	4	1.6+10	1.8+10	4.021+10	4.015+10	4.766+09	13.21
6	(^3P)	^1G	4	1.8+10	2.0+10	4.020+10	4.016+10	4.923+09	13.38
5	(^3P)	^1H	5	1.9+10	2.5+10	4.870+10	4.862+10	5.231+09	13.21
6	(^3P)	^1H	5	2.1+10	2.7+10	4.813+10	4.810+10	5.366+09	13.38