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CONTRIBUTION TO THE THEORETICAL INVESTIGATION OF ELECTRON INTERACTION WITH CARBON ATOMS IN THE DIVERTOR AND EDGE PLASMA REGIONS*

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Abstract. The fine-structure energy levels in carbon atom are calculated with the extended average level multi-configurational Dirac-Fock method in the general-purpose relativistic atomic structure package (GRASP). *D*irac *A*tomic *R*-matrix *C*ode was used to obtain the low- energy excitation cross sections of the $^3P_1$ and $^3P_2$ thresholds for the edge plasma conditions.

Key words: electron scattering, cross section, R-matrix, atomic data.

1. INTRODUCTION

A number of atomic and molecular processes take place in the fusion plasma. Specific spectral features of some processes, such as charge exchange are used as diagnostics for plasma parameters as temperature and density. Detailed data on a number of processes are required to model the plasma. Existing and future fusion devices all involve the use of hydrogen, helium, lithium, beryllium, boron, carbon, nitrogen and oxygen, and molecules of these atoms. Hydrogen isotopes constitute the fuel of fusion reactors, helium is the product of the fusion reaction, lithium is used as a beam diagnostic material, beryllium is a wall material of fusion vessels, boron is used as a coating material in fusion vessels, carbon is used in several fusion divertor plates and nitrogen is under investigation as a buffer gas in fusion devices. Light elements are the dominant impurity species in fusion research devices. Therefore, data for a number of processes for interactions among these elements are needed for design modelling of current and future fusion devices. The main populating and depopulating mechanisms of the excited energy levels of ions in divertor and edge plasmas with densities $< 10^{23} – 10^{24}$ m^{-3} are

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electron collisional excitation of the ion's ground state and radiative decay, respectively, with the majority of electron population being in the ground state of the ionization stage. Although a large number of data exist for a number of processes in several ion stages of elements of interest, significant gaps remain. Processes include electron impact excitation and ionization, radiative excitation, ionization, emission and recombination, autoionization and di-electronic recombination as well as charge exchange and heavy particle excitation and ionization. Carbon is an important contaminant of JET plasmas; it was the dominant low Z impurity before the installation of the ITER-like wall and is still present in plasma after its installation. As neutral, singly ionized C^{+}, or in molecular compounds, carbon serves as a diagnostic tool for density and temperature in fusion plasma device. Electron collisional ionization is predominantly expected to take place from one ground state to that of the next higher ionization stage. Data for electron-impact excitation of C^{2+} have been used at the EFDA-JET fusion experiment to model impurity inflow into the edge plasma from the surface with which the plasma interacts. Charge-exchange process of carbon ions with hydrogen atoms also provides a useful plasma diagnostics. A detailed knowledge of carbon transport properties, and consequently of accurate cross-section data, are required. However, the difficulties in obtaining sufficient quantities of atomic carbon in a well-defined initial state have resulted in the complete absence of experimental cross-section measurements. This absence of experimental data made theoretical investigations a computational grand challenge. In general the electron-impact excitation cross sections calculated for neutral carbon with different methods do not agree well, especially for optically forbidden transitions. For dipole-allowed transitions, the cross section is closely related to the oscillator strength, and hence the difference in the absolute values for these transitions follows the trends in the oscillator strengths calculation. There were extensive studies of astrophysically important transitions [1–4]. These authors reported oscillator strengths and transition probabilities as a further check on their structure calculations.

More extensive calculation exists for carbon ions. Theoretical works on C^{2+}, as an example, have been reported by Glass [5], Berrington [6], Berrington *et al*. [7], Mitnik *et al.* [8]. Experimental data have also been published [9]. Results from the electron and photon interactions with C^{1+} have been reported by Wilson and Bell [10], Wilson *et al.* [11, 12], Nahar [13]. There are a number of publications dealing with the ionization of the CIII to CV ionization stages. Detailed analysis of the importance of this process in populating the excited levels of ions in plasmas typical of those found in the edge of tokamak for the CIV and C V ionization stages has been recently made by Lawson *et al.* [14, and references herein].

The purpose of the present work is double. Our principal objective is to obtain the crucial information about the position, energies and radiative transition probabilities in carbon atom. Our second objective is to provide independent

predictions for the electron-impact excitations of forbidden transitions in neutral carbon, allowing for an improved assessment regarding the accuracy of the available theoretical data. The paper is structured as follows. In Section 2, after an introductory survey on the existing reported atomic data for neutral carbon, we give the results from non-relativistic and relativistic calculation of the levels energy and oscilator strengths. Comparisons between present and earlier theoretical predictions based on the *R*-matrix method and numerical procedures, are also given here. We present large scale numerical multiconfiguration Hartree-Fock (MCDF) calculation for fine-structure. Results are shown for the lowest 21 levels. Additional relativistic corrections arising from the Breit interaction and quantum electrodynamics (QED) are also included. For comparison purposes we have performed parallel calculations with the *flexible atomic code* (FAC). Section 3 is devoted to the collision problem. The full relativistic Dirac-Atomic *R*-matrix calculation is carried out to output cross sections for dominant transitions within the ground state configuration. Concluding remarks and further directions of research are presented in Section 4.

2. ATOMIC STRUCTURE CALCULATION: AN R-MATRIX APPROACH

The atomic structure problem is concerned with the computation of energy levels and rates of spontaneous transition probabilities. The R-matrix method is the most accurate technique and takes into account additional effects which may contribute on atomic quantities, like configuration interactions and relativistic effects. The ground-state configuration of carbon in the independent-particle model is $(1s)^2(2s)^2(2p)^2$, which leads to the ground-state terms ^3P, ^1D, ^1S. In neutral carbon the theoretical calculation of electron-impact excitation cross sections is made difficult by the fact that low-energy electron scattering is dominated by a resonance due to the $1s^22s^22p^3\ ^3P^0$ state of the negative ion, C^-. The theoretical prediction of the location of this resonance, and of the $1s^22s^22p^3\ ^4S^0$ and $^2D^0$ bound states of negative ion C^-, depends on a balance between short-range correlation and long range polarization effects. Different theoretical models [15–17] and numerical procedures have been used to stabilize the ground state. From these only those by Saraph [18], Rountree, Smith and Henry [19], Le Dourneuf [20], Johnson *et al.* [21] were based on the close-coupling method [22, 23] which is capable, in principle, of representing the full structure of the electronic continuum wave functions through a series of expansion in the stationary sates of the target atom. All these calculations were limited in elastic scattering from ground states and transitions amongst the $n = 2$ states at low collision energies. In the last two decades the most detailed works have been reported by Dunseath *et al.* [24], Zatsarinny *et al.* [25] and Liu, Wang and Zhou [26]. In these detailed theoretical works, close coupling calculations are performed using, respectively, the standard *R*-matrix method, *B*-spline *R*-matrix method, and the momentum space coupled-

channels optical method. Since the collision models applied are closed, the differences in the resulting cross sections and collision strengths reflect the differences in the target states description. The reported cross sections agree well in shape, but large discrepancies in magnitude exist: Dunseath's results is 32% higher than the calculation by Zatsarinny *et al*., and the results of the momentum space coupled-channels optical method are 18% lower than the calculation of *B*-spline R-matrix method.

In our work, an initial *LS*- coupling calculation has been performed. The electron correlation effects are explored by carrying out separate calculations with and without the configurations: $2s2p^3$, $2s2p^2nl$ (n = 3, 4), $2p^4$ in the target state expansion, and $2s^22p^3$, $2s2p^4$, $2s2p^3nl$ (n = 3, 4) in the (N+1)-electron wave function. For this set of calculation the RMATXI with FARM code [27] in the external region is used. The (N+1)-electron configurations data have been obtained by adding one electron to the N-electron configurations in all possible way. This wave function was augmented by including all configurations arising from virtual excitation of a 2p orbital. Exploratory calculations indicated that further 2s virtual excitations could be neglected. Results for the lowest 25 states and comparisons with existing reported data are shown in Table 1.

Table 1

Excitation energies (in eV) for the spectroscopic target states. The results are compared with experimental energy splittings from NIST, and with those reported in [23, 24]

State	Term	Present	Ref. [23]	Ref. [24]	NIST [28]
$2s^22p^2$	^3P	0.00	0.00	0.00	0.00
$2s^22p^2$	^1D	1.557	1.545	1.353	1.260
$2s^22p^2$	^1S	2.602	2.545	2.833	2.680
$2s2p^3$	$^5S^0$	3.092	3.133	4.069	4.179
$2s^22p3s$	$^3P^0$	7.401	8.488	7.488	7.481
$2s^22p3s$	$^1P^0$	7.740	8.936	7.727	7.680
$2s2p^3$	$^3D^0$	8.340	8.412	8.082	7.942
$2s^22p3p$	^1P	8.451	9.456	8.528	8.534
$2s^22p3p$	^3D	8.600	9.589	8.647	8.642
$2s^22p3p$	^3S	8.772	9.785	8.737	8.767
$2s^22p3p$	^3P	9.309	10.390	8.822	8.845
$2s^22p3p$	^1D	9.443	10.757	9.012	8.998
$2s^22p3p$	^1S	10.424	11.370	9.256	9.168
$2s2p^3$	$^3P^0$	9.517	9.981	9.504	9.326
$2s^22p3d$	$^1D^0$	9.772	10.719	9.647	9.627
$2s^22p4s$	$^3P^0$	10.142	10.810	9.708	9.683
$2s^22p4s$	$^1P^0$	9.549	10.834	9.708	9.709
$2s^22p3d$	$^3F^0$	9.517	10.809	9.729	9.695
$2s^22p3d$	$^3D^0$	9.607	10.888	9.731	9.705
$2s^22p3d$	$^1F^0$	9.607	10.947	9.759	9.732
$2s^22p3d$	$^1P^0$	9.653	10.970	9.782	9.758
$2s^22p3d$	$^3P^0$	13.407	11.018	9.983	9.830
$2s2p^3$	$^1D^0$	14.470	14.645	12.984	12.132
$2s2p^3$	$^3S^0$	13.407	15.366	13.273	13.114
$2s2p^3$	$^1P^0$	15.927	16.182	14.949	14.860

The oscillator strengths (dimensionless) are very important to obtain reliable absolute values for cross sections and rates. Table 2 presents our calculated values and comparison with the earlier published theoretical works.

Table 2

Oscillator strengths in C

Lower level	Upper level	Present	Ref. [23]	Ref. [24]	NIST [28]
$2s^22p^2\ ^3P$	$2s^22p3s\ ^3P^0$	0.124	0.154	0.133	0.140
	$2s2p^3\ ^3D^0$	0.098	0.152	0.107	0.072
	$2s2p^3\ ^3P^0$	0.028	0.117	0.055	0.063
	$2s^22p4s\ ^3P^0$	0.023	0.010	0.009	0.021
	$2s^22p3d\ ^3D^0$	0.112	0.132	0.107	0.094
	$2s^22p3d\ ^3P^0$	0.340	0.069	0.098	0.040
	$2s2p^3\ ^3S^0$	0.171	0.269	0.134	0.152
$2s^22p^2\ ^1D$	$2s^22p3s\ ^1P^0$	0.128	0.103	0.118	0.118
	$2s^22p3d\ ^1D^0$	0.009	0.007	0.013	0.013
	$2s^22p4s\ ^1P^0$	0.004	0.010	0.004	0.011
	$2s^22p3d\ ^1F^0$	0.061	0.099	0.118	0.085
	$2s^22p3d\ ^1P^0$	0.018	0.014	0.011	0.009
	$2s2p^3\ ^1D^0$	0.344	0.529	0.396	
	$2s2p^3\ ^1P^0$	0.351	0.333	0.257	
$2s^22p^2\ ^1S$	$2s^22p3s\ ^1P^0$	0.021	0.076	0.098	0.094
	$2s^22p4s\ ^1P^0$	0.007	0.001	0.004	0.005
	$2s^22p3d\ ^1P^0$	0.050	0.142	0.196	0.125
	$2s2p^3\ ^1P^0$	0.122	0.633	0.458	

Separately, we used the alternative and more satisfactory approach to treating this atomic system which is the Dirac Hamiltonian. Results for the fine-structure energy levels, the term splitting, and wave-functions composition have been obtained with the extended average level multi-configurational Dirac-Fock method (MCDF-EAL) in the general-purpose relativistic atomic structure package (GRASP). The Dirac Hamiltonian approach has the advantage that all the relativistic effects are included not only for the eigenenergies but, most importantly, in the radial wave-functions. The effect is to modify the thresholds and move the resonance structures The GRASP code is fully relativistic and is based on the *jj* coupling scheme. We have used the extended average level MCDF-EAL option where in the Hamiltonian matrix we minimize a weighted trace (proportional to $2J+1$). Additional relativistic corrections arising from the Breit interaction and quantum electrodynamics (QED) are also included. This produces a compromise set of orbitals describing closely lying states with moderate accuracy. Preliminary collision calculation has been done adopting the

Dirac atomic R-matrix code (DARC) [29, 30]. However, the code does not include the Breit and QED corrections, and hence the target energies obtained are slightly different (and comparatively less accurate) than from GRASP. Finally, for comparison purposes we have performed parallel calculations with the *flexible atomic code* (FAC) [31]. This is also fully relativistic code which provides a variety of atomic parameters, and (generally) yields results for energy levels and radiative rates comparable to GRASP. However, the differences in collision strengths between FAC and DARC can be large, particularly for forbidden transitions. Hence results from FAC are helpful in assessing the accuracy of our energy levels and radiative rates, and in estimating the contribution of resonances to effective collision strengths.

The $2s^22p^2$, $2s^22p3l$, $2s^22p4l$, $2s^22p5s$, $2p^3$ and $2p^4$ configurations of carbon give rise to 88 fine structure levels, J = 0 – 5, odd and even parity. They were included into full relativistic calculation. The calculated values were compared with the available experimental data in Atomic Structure Database of the National Institute for Standards and Technology wherever available. In Table 3 the lowest 21 levels are listed. We compare level energies obtained with GRASP (*without* and *with* the inclusion of Breit and QED effects) with the critically evaluated data compiled by NIST. In the calculation, the Dirac Coulomb contribution is the largest, with the Breit interaction introducing a significant correction. Many levels have switched when the Breit interaction is added. Also included in this table are results obtained from the FAC code (FAC) including the same CI (configuration interaction) as in GRASP. The level energies obtained without the Breit and QED effects (GRASP1) are consistently higher than the NIST values up to ~ 0.03Ryd. However, the orderings are nearly the same as those of NIST. The inclusion of Breit and QED effects (GRASP2) lowers the energies by a maximum of ~ 0.0001 Ryd. The FAC level energies are consistently lower by up to 0.003 Ryd than GRASP results, and hence are comparatively in better agreement with the NIST listings. The level ordering from FAC are also in general agreement with the calculation from GRASP, but differ in some instances, particularly for the $2s2p^3$ levels. A further inclusion of the $2p5l$, $l = 2 – 4$, configurations, labeled FAC2 calculation in Table 3 makes no appreciable difference either in the magnitude or ordering of the levels. The assessment of the uncertainty estimates is based on the comparison between the theoretical data computed within the three full relativistic structure calculations discussed above. Our final dataset will be archived in the Atomic, Molecular, Nuclear and Surface (AMNS) database (http://www.efda-itm.eu).

Table 3

The lowest 21 level energies calculation in C. NIST: http://www.nist.gov; GRASP1: energies from the GRASP code with 88 level calculations without Breit and QED effects included; GRASP2: energies from the GRASP code with 88 level calculations with Breit and QED effects; FAC1: energies from the FAC code with 88 level calculations; FAC2: energies from the FAC code with 134 level calculations

Configuration Term	*NIST NIST*	*GRASP1 (Ryd)*	*GRASP2 Grasp2*	*FAC1 FAC1*	*FAC2 FAC2*
$2s^22p^2\ {}^3P_0$	0.000	0.000	0.0000	0.00000	0.0000
$2s^22p^2\ {}^3P_1$	0.0001494	0.0001873	0.0001570	0.000064	0.000064
$2s^22p^2\ {}^3P_2$	0.0003955	0.0005584	0.0004093	0.00015105	0.000150
$2s^22p^2\ {}^1D_2$	0.09288208	0.1164040	0.1162848	0.11214485	0.112139
$2s^22p^2\ {}^1S_0$	0.1972712	0.1862982	0.1862062	0.18620175	0.185830
$2s2p^3\ {}^5S_2^0$	0.3074178	0.2209301	0.2207590	0.24012327	0.240146
$2s^22p3s\ {}^3P_0^0$	0.5497987	0.5672529	0.5670994	0.5637540	0.563779
$2s^22p3s\ {}^3P_1^0$	0.5499736	0.56743662	0.56723954	0.5638635	0.563888
$2s^22p3s\ {}^3P_2^0$	0.5503428	0.56781234	0.5673131	0.5640918	0.564117
$2s^22p3s\ {}^1P_1^0$	0.5648199	0.5915391	0.5912947	0.5898824	0.589799
$2s2p^3\ {}^3D_3^0$	0.5840030	0.6287575	0.62851954	0.6215855	0.620708
$2s2p^3\ {}^3D_1^0$	0.5840297	0.62877758	0.6286506	0.6216502	0.620772
$2s2p^3\ {}^3D_2^0$	0.5840397	0.6287918	0.6286165	0.6216703	0.620793
$2s^22p3p\ {}^1P_1$	0.6274650	0.6419229	0.6416769	0.6335048	0.632521
$2s^22p3p\ {}^3D_1$	0.6350573	0.6500307	0.6498481	0.6404025	0.639685
$2s^22p3p\ {}^3D_2$	0.6352503	0.65024712	0.6500201	0.6408055	0.640223
$2s^22p3p\ {}^3D_3$	0.6355544	0.6505814	0.65028541	0.6409477	0.640081
$2s^22p3p\ {}^3S_1$	0.6446663	0.66232293	0.6620727	0.6515510	0.651184
$2s^22p3p\ {}^3P_0$	0.6502119	0.68021956	0.6800215	0.6806422	0.680232
$2s^22p3p\ {}^3P_1$	0.6503248	0.68032504	0.6801031	0.6811181	0.680783
$2s^22p3p\ {}^3P_2$	0.6505114	0.68052371	0.6802520	0.6811958	0.680232

3. COLLISION CALCULATION

The negative ion of carbon possesses two bound states, namely the ground state $2s^22p^3\ {}^4S^0$, which is bound with respect to the $2p^2\ {}^3P$ ground state of C by 1.262 eV, and the excited state $2s^22p^3\ {}^2D^0$, whose affinity is only 0.033 eV. These bound state energies can be used to check the quality of the target wave functions and the scattering model. The third term of $2p^3$ configuration, $^2P^0$, is not bound, and it was found in many previous calculations, to occur as a shape resonance. The

most detailed previous investigation of this resonance was conducted by Johnson *et al.* [21]. We have carried out two model collision calculation. In the first, we have considered the standard *R*-matrix approach with FARM code in the external region. In this model, seven *N*-electron target states were considered, namely $1s^2 2s^2 2p^2$, $1s^2 2s 2p^3$, $1s^2 2s^2 3l$ (l = 0–2) and $1s^2 2s^2 4l$ (l = 0,1). The (N+1) configuration data included all 24 symmetries obtained by adding one electron to the *N*-electron configurations in all possible way. Total number of couplings is 312. The resonance structure as output from this model calculation is shown in Fig. 1 for the particular case of $^3P - {}^1D$ intercombination transition within the ground configuration.

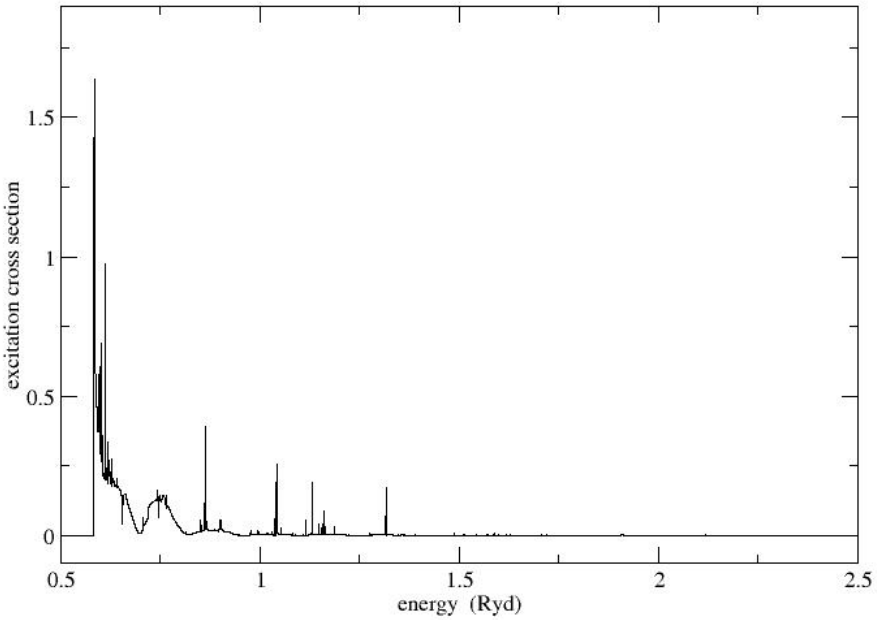

Fig. 1 – Excitation cross section (in a02) as function of collision energy (in Rydberg units) for the $^3P - {}^1D$ transition within the ground configuration of carbon.

In the second model calculation we have initiated full relativistic calculation within Dirac-Atomic R-matrix approach (DARC). Usually, results for collisional data are preferred in form of collision strengths (Ω) because it is a symmetric and dimensionless quantity. Collision strengths are related to the more commonly known collision cross section (σ_{ij}, πa_0^2) by the following relationship:

$$\Omega_{ij}(E) = k_i^2 \omega_i \sigma_{ij}(E), \tag{1}$$

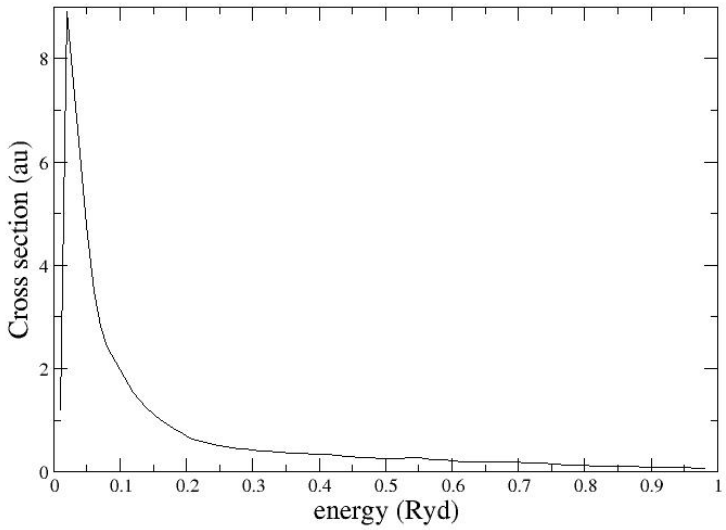

Fig. 2 – Partial cross section (in πa_0^2) for electron impact excitation of the $^3P_0 - {}^3P_1$ fine structure transition, for the $^2P_{1/2}{}^0$ threshold, in carbon, as function of collision energy [Ryd].

where k_i^2 is the incident energy of the electron and ω_i is the statistical weight of the initial state. Figure 2 shows the partial cross sections (in atomic units, 1au = πa_0^2 = = 0.88 10^{-16} cm^2) for electron impact excitation of the $^3P_0 - {}^3P_1$ transition, as function of energy (in Rydberg units), for the $^2P_{1/2}{}^0$ threshold.

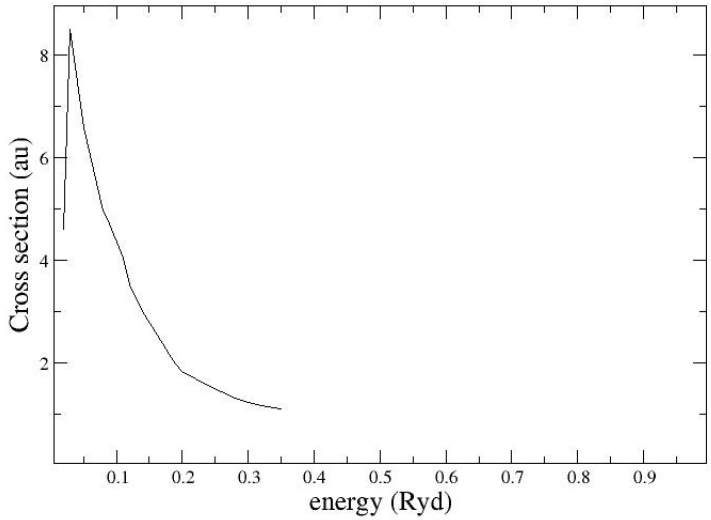

Fig. 3 – Partial cross section (in πa_0^2) for electron impact excitation of the $^3P_0 - {}^3P_1$ fine structure transition, for the $^2P_{3/2}{}^0$ threshold, in carbon, as function of collision energy [Ryd].

For the computation we have employed the DARC code, which includes the relativistic effects in a systematic way, in both the target description and the scattering model. The *R*-matrix radius adopted was 20.88 au, and 20 continuum orbitals have been included for each channel angular momentum in the expression of the wavefunction allowing to compute up to an energy of 1 Ryd. Figure 3 gives the partial cross sections for excitation of the $^3P_0$–$^3P_1$ transition, as function of energy (in Rydberg units), for the $^2P_{3/2}{}^0$ threshold. According to our results, the $^2P^0{}_{1/2}$ resonance appears in elastic scattering as a near-threshold peak at 0.02 Ryd (Fig. 2). In the calculation, this resonance manifests itself as a rapid increase in the phase shift. The energy of such resonance is often cited as the energy at which the partial cross section achieves its maximum value of the derivative of the phase shift.

4. CONCLUSIONS

The calculation reported here is part of a general theoretical investigation on the light element atoms behaviour in the divertor and edge plasma regions. In our preliminary reported work [32] the complex resonant structures in photoionization of Be-like C ions have been included through channel couplings in the R-matrix calculation. The present work refers to the particular case of electron scattering by atomic carbon. We report herein extensive non-relativistic and relativistic calculation of atomic data using new target model description. Results are in good agreement with other similar theoretical works.

The results for fine-structure energy levels, the term splitting, and the wave-functions composition are calculated with the extended average level multi-configurational Dirac-Fock method in the general-purpose relativistic atomic structure package. Energies have been computed for all levels of $2s^22p^2$, $2s2p^3$, $2p^4$, $2s^22p\ 3l$, $1s^22p4l$ and $2s^25s$ configurations. This type of calculation gives a set of 8 bound orbitals which is optimized over all the levels included. The resulting 17 relativistic orbitals produced 88 $J\pi$ levels, all of which are to be used in close-coupling expansion. Results are presented for the lowest 21 levels. Additional relativistic corrections arising from the Breit interaction and quantum electrodynamics (QED) are also included. For comparison purposes we have performed parallel calculations with the flexible atomic code (FAC). Results from FAC are helpful in assessing the accuracy of our energy levels. Our results are believed to be the first full relativistic calculation for this atomic system. The calculated values are compared with the available experimental data in Atomic Structure Database of the National Institute for Standards and Technology wherever available and a good agreement has been found.

We have calculated the excitation cross sections between 0.0001 and 1 Ryd, and within 10^{-5} Ryd of the $^3P_1$ and $^3P_2$ thresholds. Most of the calculations show a large resonance around 0.05 Ryd, due to the $1s^2 2s^2 2p^3\ ^2P^0_{1/2}$ and $^3P^0_{3/2}$ states of C^-. For comparison with threshold excitation experiments, which may eventually become possible for e-C scattering, in addition to the $^2P^0_{1/2,\ 3/2}$ resonances considered in this work, the ^4S and ^2D have to be included into the scattering calculation. This work is in progress.

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