29th EPS Conference on Plasma Phys. and Contr. Fusion Montreux, 17-21 June 2002 ECA Vol. **26B**, P-2.123 (2002)

Collision Strengths For Transitions in Ca XV

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Abstract

Collision strengths for transitions among the energetically lowest 46 fine-structure levels belonging to the ($1s^2$) $2s^22p^2$, $2s2p^3$, $2p^4$, $2s^22p3s$, $2s^22p3p$ and $2s^22p3d$ configurations of Ca XV are computed, over an electron energy range below 300 Ry, using the recent DARC program of Norrington and Grant [6]. Effective collision strengths have also been calculated at temperatures below 10^7 K, and resonances have been included. The results are compared with those available in the literature, and the accuracy of the data is assessed.

1. Introduction

In this paper we report results for collision strengths (Ω) and excitation rate coefficients for transitions among the ($1s^2$) $2s^22p^2$, $2s2p^3$, $2p^4$ and $2s^22p3\ell$ configurations of Ca XV, because calcium is an abundant element in the solar corona and chromosphere, and its emission lines have been observed in a variety of plasmas, such as: solar corona, chromosphere, prominences, and flares. Its lines are also useful in laboratory and laser plasmas for temperature and density diagnostics.

Earlier work on this ion has been performed by many workers. The prominent among these are the R-matrix calculations of Aggarwal [1], and the *Distorted-Wave* (DW) results of Bhatia and Doschek [BD: 4] and Zhang and Sampson [ZS: 7]. However, DW calculations have reported the values of Ω only at a few energies *above* thresholds, from which accurate values of rate coefficients cannot be determined, because resonances in the threshold region have not been delineated. Additionally, the ZS calculations are limited to transitions among the lowest 20 fine-structure levels of the ($1s^2$) $2s^22p^2$, $2s2p^3$ and $2p^4$ configurations, whereas BD have also included the additional 26 fine-structure levels among the ($1s^22s^22p$) 3s, 3p and 3d configurations. Our earlier calculations were also confined to the lowest 20 fine-structure levels, whereas data are also required among higher levels for diagnostic studies of solar and laboratory plasmas. Moreover, in spite of including the resonances for the computation of rates, the earlier R-matrix calculations suffer from two major deficiencies. Firstly, calculations for Ω were restricted to partial waves with angular momentum $J \leq 14.5$, and secondly, to energies below 200 Ry. The former affects the accuracy of the derived values of Ω, at higher energies, whereas the latter affects the calculations of rates, at higher temperatures. Therefore, apart from computing collision strengths for transitions among the lowest 46 fine-structure levels of the ($1s^2$) $2s^22p^2$, $2s2p^3$, $2p^4$, and $2s^22p3\ell$ configurations, we are extending the partial waves range to $J \leq 40.5$ and the energy range to 300 Ry. Thus, in present calculations we attempt to make a significant overall improvement over our earlier results.

2. Collision Strengths

Our results for energy levels, radiative rates and oscillator strengths for transitions in Ca XV have already been reported and discussed [2]. For the generation of wavefunctions, we have adopted the fully relativistic GRASP code [5]. For computations of Ω, we have employed the fully relativistic DARC program [6]. The R- matrix boundary radius has been taken to be 3.0 au, and 23 continuum orbitals have been included for

each channel angular momentum, for the expansion of the wavefunction. This allows us to compute Ω up to an energy of 300 Ry, more than sufficient for the calculation of accurate excitation rate coefficients for temperatures up to 10^7 K. We have included the contribution of all partial waves with $J \leq 40.5$, and have also included a top-up to take account of higher neglected partial waves. Additionally, to compute Ω, the diagonal elements of the continuum Hamiltonian have been adjusted in accordance with the Breit and QED corrected threshold energies. This has been done in the absence of experimental energies, which are *not* available for all the levels under consideration.

In Table 1, we list our level energies and total Ω at 3 energies of 100, 200 and 300 Ry, for transitions from the ground level to higher excited levels. A comparison made with the corresponding DW results of BD at their energies of 90 and 135 Ryd, shows agreement within 20%, except for three transitions, namely 1-9, 1-18 and 1-20, which have comparatively small magnitudes. Our values of Ω are higher by an order of magnitude for the first transition, and by a factor of two for the others. A similar comparison made with the Ω of ZS also shows an agreement within 20%, except for two transitions, namely 1-18 and 1-20, for which our results are again higher by a factor of two. Further details of the calculations and comparisons can be found in Ref. [3].

The agreement between our present RM1 and earlier RM2 [1] collision strengths is better than 20% for most of the transitions. However, for about 10% of the transitions (for example: 1-8, 2-12, and 7-16) the differences are up to 50%, and for one transition (4-13) the present results are higher by a factor of two. These differences are not surprising because RM2 calculations only included partial waves up to $J = 14.5$. Moreover, the differences for such transitions increase with the increasing energy, as expected. Therefore, the RM2 results are underestimated, particularly towards the higher end of the energy range. However, now we have excellent agreement between our present R-matrix [RM1] and earlier DW results at all energies. This is in spite of the fact that the RM1 and ZS calculations are in the jj coupling scheme, while the BD are in the LSJ coupling scheme.

3. Effective Collision Strengths

Effective collision strengths (Υ) are obtaiined after averaging the Ω data over a Maxwellian distribution of electon energies, and are very simply related to the excitation and de-excitation rate coefficients. In order to resolve resonances in threshold region we have adopted an energy mesh of better than 0.002 Ry. In Table 2 we present our *preliminary* results at three representative temperatures of 10^5, 10^6 and 10^7 K for transitions among the levels of the $1s^2 2s^2 2p^2$ ground configuration. Our earlier RM2 results are also included in this table for the sake of comparison. Differences between the two sets of Υ are up to a factor of two (see, for example, transitions 1-3 and 1-4). These differences are to be analysed in detail, but are mainly due to the improvements made in the present calculations, as discussed earlier. A complete set of results for both Ω as well Υ along with detailed comparisons will soon be reported.

4. Conclusions

Collision strengths and effective collision among the lowest 46 fine-structure levels of Ca XV have been computed in a wide energy/temperature range. Our present computations are not only an extension of our earlier work [1], which reported Ω for transitions among the 20 fine-structure levels of the $(1s^2)\ 2s^2 2p^2$, $2s2p^3$ and $2p^4$ configurations,

Table 1. Level energies and Collision Strength for resonance transitions of Ca XV.

Index	Configuration	Level	Energy	100	200	300 (Ry)
2	$1s^2 2s^2 2p^2$	$^3P_1$	0.1601	8.123-3	3.369-3	1.858-3
3	$1s^2 2s^2 2p^2$	$^3P_2$	0.3281	1.552-2	1.535-2	1.556-2
4	$1s^2 2s^2 2p^2$	$^1D_2$	1.0138	2.814-3	1.186-3	7.180-4
5	$1s^2 2s^2 2p^2$	$^1S_0$	1.7695	2.673-4	8.196-5	3.760-5
6	$1s^2 2s 2p^3$	$^5S_2{}^o$	2.3928	1.501-3	6.281-4	3.400-4
7	$1s^2 2s 2p^3$	$^3D_2{}^o$	4.5364	1.289-3	5.490-4	2.996-4
8	$1s^2 2s 2p^3$	$^3D_1{}^o$	4.5456	3.602-1	4.191-1	4.508-1
9	$1s^2 2s 2p^3$	$^3D_3{}^o$	4.5677	1.529-5	9.916-6	7.868-6
10	$1s^2 2s 2p^3$	$^3P_0{}^o$	5,3144	8.901-5	3.665-5	1.953-5
11	$1s^2 2s 2p^3$	$^3P_1{}^o$	5.3246	1.698-1	1.983-1	2.132-1
12	$1s^2 2s 2p^3$	$^3P_2{}^o$	5.3500	2.958-4	1.257-4	6.919-5
13	$1s^2 2s 2p^3$	$^3S_1{}^o$	6.7940	1.610-1	1.890-1	2.041-1
14	$1s^2 2s 2p^3$	$^1D_2{}^o$	6.7971	5.828-4	2.438-4	1.320-4
15	$1s^2 2s 2p^3$	$^1P_1{}^o$	7.5695	2.300-4	1.651-4	1.482-4
16	$1s^2 2p^4$	$^3P_2$	10.2321	6.838-4	6.777-4	6.910-4
17	$1s^2 2p^4$	$^3P_1$	10.4681	5.220-6	1.537-6	6.750-7
18	$1s^2 2p^4$	$^3P_0$	10.5269	2.841-4	2.359-4	2.116-4
19	$1s^2 2p^4$	$^1D_2$	11.1048	1.733-5	5.230-6	2.362-6
20	$1s^2 2p^4$	$^1S_0$	12.5692	1.148-5	8.186-6	6.995-6
21	$1s^2 2s^2 2p 3s$	$^3P_0{}^o$	37.4440	1.562-4	4.975-5	2.377-5
22	$1s^2 2s^2 2p 3s$	$^3P_1{}^o$	37.4905	3.550-3	6.124-3	7.973-3
23	$1s^2 2s^2 2p 3s$	$^3P_2{}^o$	37.7821	8.654-5	2.662-5	1.255-5
24	$1s^2 2s^2 2p 3s$	$^1P_1{}^o$	37.9481	2.080-4	2.868-4	3.600-4
25	$1s^2 2s^2 2p 3p$	$^3D_1$	38.5909	8.030-4	2.682-4	1.367-4
26	$1s^2 2s^2 2p 3p$	$^3D_2$	38.8009	3.409-3	4.172-3	4.616-3
27	$1s^2 2s^2 2p 3p$	$^1P_1$	38.8099	6.181-4	2.010-4	9.901-5
28	$1s^2 2s^2 2p 3p$	$^3D_3$	39.0419	1.914-4	5.995-5	2.860-5
29	$1s^2 2s^2 2p 3p$	$^3S_1$	39.0900	1.903-4	6.685-5	3.741-5
30	$1s^2 2s^2 2p 3p$	$^3P_0$	39.1045	2.814-2	3.007-2	3.092-2
31	$1s^2 2s^2 2p 3p$	$^3P_1$	39.2720	4.012-4	1.402-4	7.242-5
32	$1s^2 2s^2 2p 3p$	$^3P_2$	39.3384	6.941-4	6.163-4	6.309-4
33	$1s^2 2s^2 2p 3p$	$^1D_2$	39.6112	2.640-4	1.023-4	6.842-5
34	$1s^2 2s^2 2p 3d$	$^3F_2{}^o$	39.9878	1.229-3	3.129-4	1.372-4
35	$1s^2 2s^2 2p 3p$	$^1S_0$	40.0342	9.583-5	6.670-5	6.185-5
36	$1s^2 2s^2 2p 3d$	$^3F_3{}^o$	40.1271	3.675-3	4.189-3	4.501-3
37	$1s^2 2s^2 2p 3d$	$^1D_2{}^o$	40.1990	1.744-3	4.781-4	2.139-4
38	$1s^2 2s^2 2p 3d$	$^3F_4{}^o$	40.3352	2.647-4	6.867-5	3.041-5
39	$1s^2 2s^2 2p 3d$	$^3D_1{}^o$	40.3696	1.351-1	2.005-1	2.442-1
40	$1s^2 2s^2 2p 3d$	$^3D_2{}^o$	40.4639	5.841-4	1.525-4	6.678-5
41	$1s^2 2s^2 2p 3d$	$^3D_3{}^o$	40.5834	7.294-4	6.088-4	6.107-4
42	$1s^2 2s^2 2p 3d$	$^3P_2{}^o$	40.6537	1.527-4	4.157-5	2.012-5
43	$1s^2 2s^2 2p 3d$	$^3P_1{}^o$	40.6719	1.004-3	1.261-3	1.483-3
44	$1s^2 2s^2 2p 3d$	$^3P_0{}^o$	40.6853	8.600-5	2.509-5	1.155-5
45	$1s^2 2s^2 2p 3d$	$^1P_1{}^o$	41.0566	1.285-3	1.672-3	1.997-3
46	$1s^2 2s^2 2p 3d$	$^1F_3{}^o$	41.0685	4.208-4	1.019-4	4.386-5

but are also an improvement over those results. The major improvements are the extension of the energy range up to 300 Ry, which was restricted to 200 Ry earlier, and the inclusion of a higher range of partial waves (up to $J = 40.5$ in comparison to the earlier 14.5). The latter factor particularly improves the accuracy of Ω for allowed transitions, and at high energies. As a result of this, the present R-matrix results are in excellent agreement with earlier DW calculations, for a majority of transitions. However, for a few forbidden transitions (such as 0-0 and 0-3) the differences are still up to a factor of two, but the magnitude of Ω for such transitions are negligibly small. Based on the comparisons made between our present and earlier available R-matrix and DW results, and our experience of similar calculations on other ions, we can say with confidence that the presently computed values of Ω are accurate to within 10% for all transitions and at all energies. Accuracy of Υ values is yet to be assessed.

Table 2. Comparison between present [RM1] and earlier RM2 [1] results of effective collision strengths for transitions within the levels of the $1s^2 2s^2 2p^2$ ground configuration of Ca XV. ($a \pm b \equiv a \times 10^{\pm b}$).

T_e (log K)		5.0	5.0	6.0	6.0	7.0	7.0
Transition	I-J	RM1	RM2	RM1	RM2	RM1	RM2
$^3P_0$ - $^3P_1$	1-2	1.723-1	1.679-1	1.396-1	1.743-1	4.165-2	3.872-2
$^3P_0$ - $^3P_2$	1-3	7.092-2	1.211-1	7.301-2	2.430-1	2.980-2	5.157-2
$^3P_0$ - $^1D_2$	1-4	6.764-2	4.178-2	3.302-2	2.187-2	1.300-2	7.742-3
$^3P_0$ - $^1S_0$	1-5	2.057-2	1.327-2	8.828-3	7.203-3	3.313-3	1.493-3
$^3P_1$ - $^3P_2$	2-3	3.287-1	5.386-1	3.473-1	8.777-1	1.214-1	1.911-1
$^3P_1$ - $^1D_2$	2-4	2.149-1	1.555-1	1.456-1	9.186-2	5.636-2	3.181-2
$^3P_1$ - $^1S_0$	2-5	4.250-2	3.104-2	2.303-2	1.797-2	1.075-2	4.974-3
$^3P_2$ - $^1D_2$	3-4	4.330-1	3.899-1	2.342-1	3.602-1	1.095-1	1.001-1
$^3P_2$ - $^1S_0$	3-5	3.875-2	4.975-2	2.681-2	3.220-2	1.504-2	9.405-3
$^1D_2$ - $^1S_0$	4-5	2.162-1	2.105-1	1.066-1	9.690-2	5.773-2	4.982-2

This work has been financed by EPSRC and PPARC of UK, and we wish to thank Dr. Patrick Norrington for providing his code available to us prior to publication.

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