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Excitation Rates for Transitions in Fe XI

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Abstract

Energy levels and radiative rates for transitions among the lowest 48 fine-structure levels belonging to the ($1s^22s^22p^6$) $3s^23p^4$, $3s3p^5$, $3s^23p^33d$ and $3p^6$ configurations of Fe XI have been calculated using the fully relativistic GRASP code. Additionally, collision strengths and excitation rates for transitions among these levels have also been computed using the DARC program. Energy levels are assessed to be accurate to better than 10% for a majority of levels, while oscillator strengths, collision strengths and excitation rates for all transitions should be reliable to better than 20%.

1. Introduction

For the interpretation of observational spectroscopic data, theoretical results for energy levels, radiative rates, collision strengths, rate coefficients, etc. are required, as the corresponding experimental data are often not available, except for energy levels. Emission lines of Fe XI have been observed in UV and EUV range of the solar spectrum, as well as in late-type stars. Hence, in this paper we report our results for the above mentioned parameters.

For performing our calculations, we have adopted the GRASP code [3] for generating wavefunctions and the DARC program [8] for computing collision strengths (Ω). Energy levels, radiative rates and Ω have been computed for transitions among the lowest 48 fine-structure levels belonging to the ($1s^22s^22p^6$) $3s^23p^4$, $3s3p^5$, $3s^23p^33d$ and $3p^6$ configurations, but configuration interaction (CI) has also been included with the levels of the $3s^23p^23d^2$, $3s^23p^34s$, $3s^23p^34p$ and $3s^23p^34d$ configurations. Collision strengths have been computed in a wide energy range below 100 Ry, and a mesh better than 0.002 Ry has been adopted in the threshold region, in order to account for resonances in the calculations of effective collision strengths Υ, which are obtained after averaging the Ω data over a Maxwellian distribution of electron velocities. Results for Υ have been obtained in a wide temperature range below 5×10^6 K, suitable for plasma applications.

Earlier results for Fe XI have been obtained by Tayal and co-workers [GT: 5-6] and Bhatia and Doschek [BD: 1], who have adopted the CIV3 [7] and SuperStructure (SS: 4) programs for the generation of wavefunctions, and the Breit-Pauli R-matrix (BPRM: 9) and Distorted-Wave (DW) programs, respectively, for the computation of Ω. Therefore, their calculations are in the semi-relativistic LSJ coupling scheme, whereas we have adopted the fully relativistic jj coupling scheme. BD have reported the values of Ω at only three energies, i.e. 8, 16 and 24 Ry, whereas GT have also tabulated results for Υ. But their calculations have been performed for transitions among a subset (38 levels) of the above levels, although energy levels and radiative rates have been computed among the lowest 47 fine-structure levels [2]. Since the remaining 9 levels ($^5D^o_{0,1,2,3,4}$, $^3G^o_{3,4,5}$ and $^1G^o_4$) lie *below* the highest threshold of their calculations, they have clearly not included the resonances arising from these levels, and perhaps therefore have underestimated the values of Υ for a majority of transitions. The other excluded ($3p^6$ $^1S_0$) level is also just above the other remaining levels (see Table 1 of [1]), and therefore its omission is not justified in any accurate calculation. Hence, we strongly believe that there is enough scope to extend as well as to improve upon their results.

2. Energy Levels and Radiative Rates

The ($1s^22s^22p^6$) $3s^23p^4$, $3s3p^5$, $3s^23p^33d$ and $3p^6$ configurations of Fe XI give rise to 48 fine-structure levels. To calculate level energies and radiative rates, we have adopted the GRASP code [3]. However, Fe XI is an ion for which CI is equally important. Therefore, based on our test calculations, we have also included CI among the additional $3s^23p^23d^2$, $3s^23p^34s$, $3s^23p^34p$ and $3s^23p^34d$ configurations. On the other hand, SS calculations [1] include CI among the first 4 basic configurations only, but the CIV3 calculations [2] include elaborate CI involving all 4ℓ orbitals.

Different theoretical calculations show slightly different energy levels order. Our theoretical and experimentally compiled energy levels of NIST agree to better than 10%, except for $3s^23p^4\ ^1S_0$, for which our energy is lower by 15%. The energies of the CIV3 calculations [2] are in better agreement with the measurements, but their energy order is different in a few instances. Similarly, the level order of the SS calculations [1] is entirely different from both the theoretical as well as experimental energy order. However, the differences between various theoretical results are within ~10%.

Our GRASP radiative rates agree within 50% for a majority of strong transitions with those from CIV3 [2] and SS [1] calculations. Since all three calculations employ different amount of CI in the generation of wavefunctions, differences among the three sets are expected. However, for transitions involving levels 39 and 41 ($3s^23p^33d\ ^3P^o_1$ and $^1P^o_1$), differences between our GRASP and the CIV3 and SS f- values are unexpectedly large. It appears that these two levels have been interchanged in the other two calculations.

3. Collision Strengths

For the computations of Ω, we have used the DARC program [8]. This is based on the jj coupling scheme, and uses the Dirac-Coulomb Hamiltonian in the R- matrix approach. The R-matrix radius has been adopted to be 5.4 au, and 25 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 100 Ry. All partial waves with $J \leq 40.5$ have been included, and for the convergence of allowed transitions a top-up, based on the sum rules, has also been included.

The differences among the three sets of Ω are up to a factor of 5 for some transitions, such as 2-41 and 2-45. Differences between our present R-matrix and the earlier DW calculations are less than 50%, and are in accordance with the corresponding f- values. But the reported values of Ω from GT appear to be incompatible with their known values of oscillator strengths. For example, for the 1-37 transition the f- value of GT is about 25% higher than that of BD, but the two sets of Ω are comparable at all three energies. Similarly, for the 2-45 transition the f- value of GT is about 30% lower than that of the other two calculations, but their values of Ω are lower by a factor of four.

In Table 1 we list and compare our values of Υ with those of GT for 10 fine-structure transitions within the levels of the $3s^23p^4$ configuration at four representative temperatures of 10^4, 10^5, 10^6 and 5×10^6 K. Our Υ results are *higher* than those of GT by over a factor of two at the lowest temperature for the 1-2 ($^3P_2$-$^3P_1$) and 1-3 ($^3P_2$-$^3P_0$) transitions, but are *lower* by nearly the same factor of two for the 1-4 ($^3P_2$-$^1D_2$) transition. This large difference in the two sets of Υ quickly disappears as temperature increases. This is mainly because of the presence (or absence) of near-threshold resonances. Furthermore, the resolution of GT data is coarser i.e. 0.005 Ry in comparison to our better than 0.002 Ry. This coarser mesh can obviously affect the results significantly by either omitting many of the resonances or accounting for their larger widths.

Table 1. Effective collision strengths for transitions among the levels of the $1s^2 2s^2 2p^6 3s^2 3p^4$ configuration of Fe XI. ($a \pm b \equiv a \times 10^{\pm b}$).

Transition	DARC				BPRM [5-6]			
T_e (K)	10^4	10^5	10^6	5×10^6	10^4	10^5	10^6	5×10^6
$^3P_2$-$^3P_1$	2.260-0	2.241-0	1.456-0	5.571-1	9.07-1	2.10-0	1.42-0	4.69-1
$^3P_2$-$^3P_0$	5.563-1	5.360-1	3.257-1	1.632-1	2.42-1	5.02-1	3.28-1	1.26-1
$^3P_2$-$^1D_2$	1.022-0	1.515-0	8.043-1	2.683-1	1.95-0	1.69-0	8.93-1	2.86-1
$^3P_2$-$^1S_0$	1.755-1	1.557-1	7.596-2	2.135-2	1.72-1	2.05-1	9.65-2	2.77-2
$^3P_1$-$^3P_0$	5.246-1	5.957-1	4.657-1	1.369-1	5.25-1	6.79-1	5.19-1	1.49-1
$^3P_1$-$^1D_2$	6.366-1	1.054-0	6.359-1	1.878-1	8.40-1	9.93-1	5.64-1	1.68-1
$^3P_1$-$^1S_0$	1.366-1	1.313-1	7.097-2	2.037-2	1.21-1	1.98-1	9.78-2	2.81-2
$^3P_0$-$^1D_2$	3.131-1	3.753-1	2.268-1	7.449-2	2.77-1	3.39-1	2.03-1	6.22-2
$^3P_0$-$^1S_0$	6.854-2	9.359-2	5.349-2	1.445-2	1.10-1	1.82-1	9.67-2	3.68-2
$^1D_2$-$^1S_0$	6.226-1	6.178-1	4.909-1	3.869-1	7.24-1	7.49-1	5.35-2	2.94-1

For other transitions, such as 2-3,4,5 and 3-4, differences between the two sets of Υ are restricted to less than 50%. However, the differences persist in the entire temperature range and are due to our better resolution of resonances and a higher range of energy for Ω. Similarly the two calculations consistently differ in the entire temperature range for the $^3P_0$ - $^1S_0$ (3-5) transition, and the GT results are higher by a factor of two.

For transitions among the higher levels, the Ω and Υ values of GT are comparable at $T_e = 5.0\times10^5$ K, but at $T_e = 3.0\times10^6$ K, the Υ values are lower up to 25%. The difference between their Ω and Υ values increases with increasing electron temperature. This is *not* compatible with their results for Ω, and indicates an error in their calculations of Υ. This is because they have computed the Ω values up to E = 40 Ry only, which is not sufficient for the convergence of the Maxwellian integral. This is the main reason that we have performed our calculations up to an energy of 100 Ry, so that values of Υ can be safely determined up to a temperature of $\sim 5\times10^6$ K, suitable for applications in astrophysical, laser and fusion plasmas.

Finally, in Table 2, we present the rates from the ground configuration ($1s^2 2s^2 2p^6 3s^2 3p^4$) to four excited levels of the $3p^3 3d$ ($^1F^o_3$, $^3D^o_1$, $^1D^o_2$ and $^3P^o_2$) and two levels ($^3P^o_1$ and $^1P^o_1$) of the $3s3p^3$ configurations. The corresponding available rates of GT and BD are also included in this table, and so are the experimental results of Wang et al [10].

The difference between the experimental and theoretical rates is over a factor of two. The BD rates are in closest agreement with the experimental rates, and the differences are within 50% except for the $^3P^o_1$ level. However, this close agreement is misleading as the dominant contribution in these rates come from the strong allowed transitions (for example, 4-46 ($3s^2 3p^4$ $^1D_2$ - $3s^2 3p^3 3d$ $^1F^o_3$) transition for the $^1F^o_3$ level rates), for which the f- values and subsequently the Ω values of BD are overestimated. The discrepancy between our theoretical and available experimental rates is also of $\sim$ 50%, except for the $^1D^o_2$ level for which our rates are lower by a factor of two. However, Wang et al have assessed their rates to be overestimated by a factor of 1.5 - 2.0. With this assessment, the theory and experiment agree well.

Table 2. Comparison of experimental and theoretical excitation rates (in 10^{-9} cm^3 s^{-1}) at electron temperature of 160 eV for transitions from the levels of the ground configuration ($1s^22s^22p^63s^23p^4$) to $^1F^o_3$, $^3D^o_1$, $^1D^o_2$, and $^3P^o_2$ levels of the $3p^33d$ configuration, and $^3P^o_1$ and $^1P^o_1$ levels of the $3s3p^3$ configuration..

		$3p^33d$ configuration				$3s3p^3$ configuration	
Method	Reference	$^1F^o_3$	$^3D^o_1$	$^1D^o_2$	$^3P^o_2$	$^3P^o_1$	$^1P^o_1$
Expt.	[10]	3.7	1.6	2.4	3.1	0.75	0.66
DARC	Present	2.75	1.06	1.25	2.03	0.45	0.63
BPRM	[5-6]	2.2	1.0	1.4	1.7	0.34	0.56
DW	[1]	3.38	1.34	1.77	2.63	0.43	0.59

4. Conclusions

In this paper we have obtained a consistent set of results for energy levels, radiative rates, collision strengths and excitation rate coefficients for transitions in Fe XI. Relativistic effects, CI, a large range of partial waves and electron energy, and resonances in a fine energy mesh have been included in the calculations. All these factors are a significant improvement over the available comparable results of GT. Our calculated values of collision strengths are expected to be accurate to within 10% at energies below 25 Ry, but may be inaccurate up to 20% at higher energies for a few allowed transitions. A complete set of results for both Ω and Υ along with detail comparisons will soon be reported.

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