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Excitation Rates for Transitions in Fe XIII

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Abstract

Effective collision strengths for transitions among the lowest 97 fine-structure levels belonging to the ($1s^2 2s^2 2p^6$) $3s^2 3p^2$, $3s3p^3$, $3s^2 3p3d$, $3p^4$, $3s3p^2 3d$ and $3s^2 3d^2$ configurations of Fe XIII have been calculated using the fully relativistic Dirac Atomic R-matrix Code. Resonances have been resolved in the threshold region, and results are reported over a wide electron temperature range below $\log T_e = 6.8$ K. The accuracy of the data is assessed to be $\sim 20\,\%$.

Keywords:

effective collision strength, excitation rate

1. Introduction

Electron impact excitation of iron ions has been a subject of intense research because iron is an abundant element, particularly in solar and fusion plasmas, and its lines are observed in almost all ionization stages. Emission lines of Fe XIII have been observed in the UV and EUV ranges of the solar spectrum, as well as in late-type stars. Almost all of its observed lines, whether in the Sun or other stars, have proved excellent tools for density diagnostics at coronal temperatures. The interpretation of the vast amount of observations requires theoretical data for atomic parameters, such as energy levels, radiative rates, collision strengths, and rate coefficients, because experimental results for these are generally not available. Results for energy levels, radiative rates, and collision strengths for transitions among the lowest 97 fine-structure levels belonging to the ($1s^2 2s^2 2p^6$) $3s^2 3p^2$, $3s3p^3$, $3s^2 3p3d$, $3p^4$, $3s3p^2 3d$ and $3s^2 3d^2$ configurations of Fe XIII were recently reported by us [1], and in this work we present our results for excitation rate coefficients.

Earlier calculations for Fe XIII have been performed by many workers, but the most recent and comprehensive results available today are those of Gupta & Tayal (GT: [2]). They have reported energy levels, radiative rates, and collision strengths (Ω) for transitions among 26 fine-structure levels of the $3s^2 3p^2$, $3s3p^3$ and $3s^2 3p3d$ configurations. Furthermore, they have resolved resonances in thresholds region and have reported results for effective collision strengths (Υ) at temperatures below 5×10^6 K, which is sufficient for applications in plasma diagnostics. In their calculations they have included configuration interaction (CI) for generating wavefunctions, and one-body relativistic operators for calculating Ω. Therefore, their results should be the most reliable available today. However, in a recent paper Landi [3] has emphasized a need for fresh calculations, because electron densities derived from line ratios calculated from the recent atomic data of GT and earlier data of Fawcett & Mason (FM: [4]) differ by a factor of two, and hence provide different results for plasma diagnostics. Therefore, our aim is to assess the accuracy of the available atomic data, and we achieve it by performing an independent calculation.

We have adopted the GRASP and DARC programs for the computations of wavefunctions and Ω, respectively. Thus our calculations are fully relativistic in the jj coupling scheme. Our results of Ω were in broad agreement with those of GT, and the differences, if any, were in accordance with the wavefunctions, i.e. the f- values. However, the corresponding results of FM were found to be deficient. For forbidden transitions, their values of Ω are *underestimated*, whereas for the allowed transitions they are *overestimated*. Additionally, for some of the allowed transitions their results of Ω are *not* in accordance with their corresponding f- values. Since our calculations for Ω in thresholds region are now complete, below we compare our Υ results with those of GT.

2. Effective collision strengths

Since the threshold region is dominated by resonances, we have computed values of Ω at over 6760 energies with a fine mesh of ≤ 0.002 Ry. In Fig. 1 we show resonances for only the ($3s^2 3p^2$) $^3P_0$ - $^3P_2$ (1-3) transition, which gives enough idea about the density and im-

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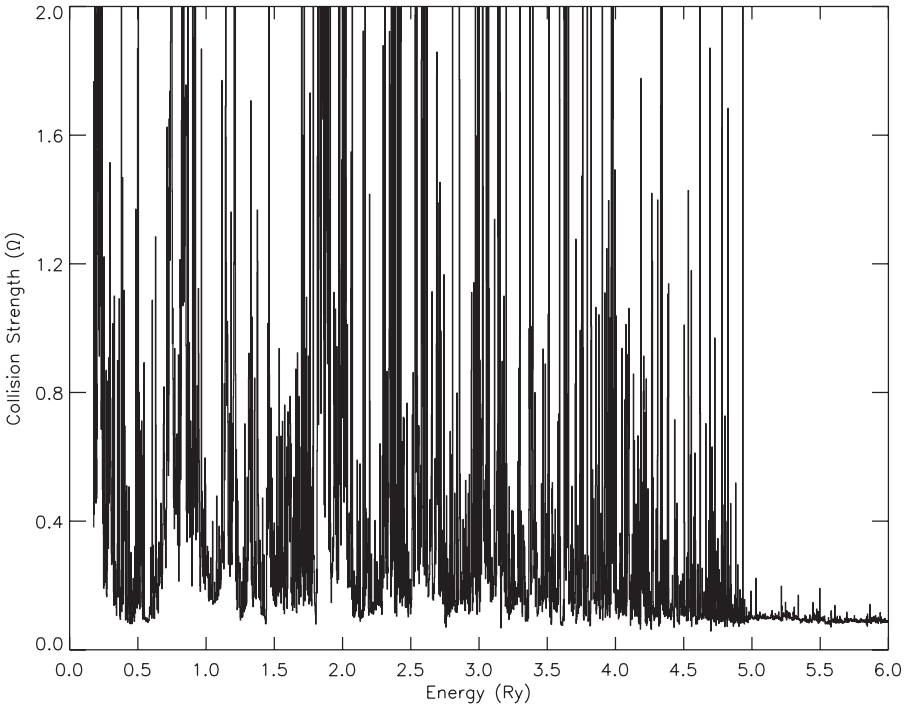

Fig. 1 Collision strengths for the $(3s^2 3p^2)\ ^3P_0$-$^3P_2$ (1-3) transition of Fe XIII

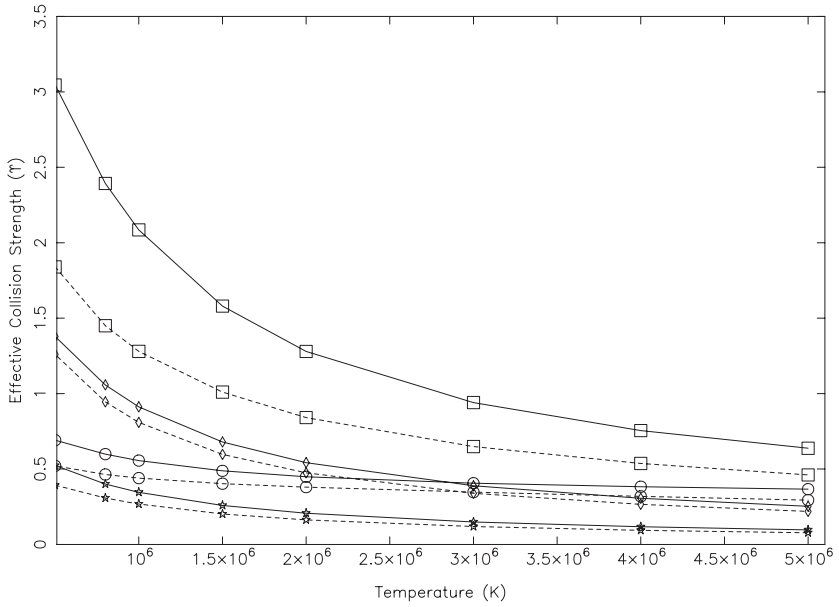

Fig. 2 Effective collision strengths (Υ) for some transitions within the $3s^2 3p^2$ configuration of Fe XIII. Continuous curve: present results, broken curve: Gupta & Tayal [2], stars: $^3P_0$-$^3P_1$ (1-2), diamonds: $^3P_0$-$^1D_2$ (1-4), squares: $^3P_2$-$^1D_2$ (3-4), and circles: $^1D_2$-$^1S_0$ (4-5)

portance of resonances. The values of Υ are computed at a series of electron temperatures in the range $5.0 \leq \log T_e \leq 6.8$ K, which is fully sufficient for the application of the data in solar, astrophysical and fusion plasmas. A complete set of results for all transitions (among all 97 levels) along with detailed comparisons is available elsewhere [5], but below we compare in Fig. 2 our results of Υ with those of GT, for some of the transitions within the $3s^2 3p^2$ configuration.

For all the four transitions shown in Fig. 2, our present results of Υ are higher than those of GT, at all temperatures. Our higher values of Υ at lower temperatures are because of the denser resonances observed in our calculations, which are in the jj coupling scheme in which *fine-structure* is included in the definition of channel coupling. This procedure accounts for the resonances more accurately in comparison to the *LS J* coupling scheme adopted by GT. Additionally, the energy

mesh in our calculations is finer (better than 0.002 Ry) in comparison to the coarse mesh of 0.005 Ry of GT. This particularly affects the results when the magnitude of Ω is high for the near-threshold resonances, as shown in Fig. 1. Similarly, our results of Υ continue to be higher at higher temperatures, because GT have reported their values of Υ up to a temperature of 5×10^6 K, which amounts to $\sim$ 32 Ry in energy units. However, they have computed values of Ω up to an energy of 60 Ry only, which is *not* sufficient for the calculations of Υ at higher temperatures. As a result of this, their values of Υ are *underestimated* towards the higher end of the temperature range. Furthermore, this limited energy range of their calculations of Ω affects the values of Υ more for the allowed transitions, than the forbidden ones. This can be easily confirmed by a closer look at their results of Ω in their Table 4 for transitions, such as $3s^23p^2\ ^3P_0$ - $3s^23p3d\ ^3P^o_1$, $3s^23p^2\ ^3P_1$ - $3s^23p3d\ ^1D^o_2$, $3s^23p^2\ ^3P_2$ - $3s^23p3d\ ^3D^o_2$, $3s^23p^2\ ^1D_2$ - $3s^23p3d\ ^1F^o_3$, and $3s^23p^2\ ^1S_0$ - $3s^23p3d\ ^1P^o_1$, for which values of Ω increase with increasing energy (in both calculations), as these are allowed transitions. However, for all of these (and many more) transitions their corresponding results of Υ *decrease* with increasing temperature as seen in their Table 5.

To conclude, we have reported results for Υ, which are very simply related to the excitation rate coefficients. Relativistic effects and CI have been included while generating the wavefunctions, and resonances have been delineated in a fine energy mesh to account for their contribution. Apart from performing our calculations in the jj coupling scheme, we have attempted to make an overall improvement over the existing results of GT. These improvements have mainly been achieved by the inclusion of: (i) a larger number of levels, i.e. 97 in comparison to the 26 of GT, (ii) a wider range of partial waves, i.e. $J \leq 39.5$ in comparison to the $J \leq 22.5$ of GT, and (iii) a higher range of energy, i.e. 120 Ry in comparison to the 60 Ry of GT. Additionally, results for all relevant atomic parameters are now reported for a larger number of transitions than previously available. Based on several comparisons, accuracy of our present results is assessed to be $\sim$ 20 %, but scope remains for improvement, mainly by including additional CI in the generation of wavefunctions. Similarly our results of Υ, particularly towards the lower end of the temperature range, are likely to be variable due to the presence (or absence) of large and dense near-threshold resonances, for which some experimentation with decreasing energy mesh may also be useful.

It is unfortunate that both sets of atomic data (of FM and GT) adopted by Landi (2002) in his detailed analysis of observational data are found to be deficient, and any agreements observed between experimental observations and theoretical determinations from their data appear to be fortuitous. Therefore, a fresh analysis of observational astrophysical data in conjunction with the present atomic data should be of considerable interest.

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