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Effective collision strengths for optically allowed transitions among degenerate levels of hydrogenic ions with $2 \leqslant Z \leqslant 30$

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ABSTRACT

The Coulomb–Born approximation is used to calculate electron-impact excitation collision strengths and effective collision strengths for optically allowed transitions among degenerate fine-structure levels of hydrogenic ions with $2 \leqslant Z \leqslant 30$ and $n \leqslant 5$. Collision strengths are calculated over a wide range of energies up to $E_j/Z^2 = 10$ Ryd. Effective collision strengths are obtained over a wide temperature range up to 10^8 K by integrating the collision strengths over a Maxwellian distribution of electron velocities.

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Contents

1. Introduction

Atomic data for many parameters (such as energy levels, radiative rates, and electron impact excitation rates) are required for the modeling of a variety of plasmas, such as astrophysical, solar, laser, and fusion plasmas. Such data are also needed in plasma diagnostics, for determining density, temperature, and chemical composition. Emission lines of many H-like ions, including C VI, O VIII, Mg XII, Ca XX, and Fe XXVI, have been observed in the solar and other astrophysical plasmas [1]. However, there is paucity of atomic data for these ions in the literature, both theoretical and experimental, particularly for the collision strengths (Ω) and effective collision strengths (Υ). The available theoretical data for Υ are limited either to a few ions or a few levels. For example, Ballance et al. [2] have reported results for Υ for seven ions up to $Z = 10$, but their calculations are only in *LS* coupling, whereas it is the fine-structure transitions which are observed spectroscopically. However, Ballance et al. [3] have reported Υ results for fine-structure transitions in Fe XXVI, but their available data for Υ were incomplete as optically allowed transitions among the degenerate levels of a state, such as $2s_{1/2} - 2p_{1/2}$ and $3p_{1/2} - 3d_{1/2}$, were missing. This is because such transitions have very small energies, and hence converge very slowly with increasing partial waves, as demonstrated by Igarashi et al. [4,5] for transitions of the $n = 2$ levels of He II, C VI, and Ar XVIII. We will refer to these transitions as 'elastic' because of their very small energies. We also note that Ballance et al. have now included these elastic transitions in the results posted on their website http://www-cfadc.phy.ornl.gov/home.html.

Adopting a close coupling (CC) approximation, Zygelman and Dalgarno [6] reported values of Ω and Υ for some hydrogenic ions, namely He II, C VI, Mg XII, S XVI, and Ar XVIII, but only for elastic transitions within the $n = 2$ levels. Therefore, there is a clear need to extend such data for elastic transitions among the higher excited levels of hydrogenic ions. Additionally, through a variety of calculations, Igarashi et al. [4,5] demonstrated that values of Ω obtained from the CC approximation and a comparatively simple Coulomb–Born (CB) approximation [7] are comparable over a wide energy range for the elastic transitions, but latter calculations significantly reduce the computational effort by about a factor of 50. Therefore, adopting the CB approximation of Burgess et al. [7] in the code developed by Igarashi et al., Aggarwal et al. [8–10] recently reported a complete set of results for both Ω and Υ for *all* transitions among the $n \leqslant 5$ levels of Al XIII, Ar XVIII, and Fe XXVI. However, corresponding data are required for many ions as recently emphasized by Aggarwal and Keenan [11]. In this paper we report values of Ω and Υ for all hydrogenic ions with $2 \leqslant Z \leqslant 30$ and for all the 26 elastic transitions within the $n \leqslant 5$ levels.

The present calculations for Ω are based on the partial wave expansion method, as described in detail by Igarashi et al. [4,5]. However, we note that the CB approximation can also be expressed analytically and has therefore been implemented in electron-ion scattering codes such as FAC [12] and HULLAC [13]. It has also been recently implemented in the Dirac Atomic R-matrix Code (DARC) of Norrington and Grant [14], but only at energies above all the thresholds. Therefore, although the calculations from DARC and CB codes provide comparable values of Ω for many transitions, as recently demonstrated by Aggarwal et al. [8–10] for Al XIII, Ar XVIII, and Fe XXVI, at present the corresponding results obtained for Υ values from DARC will be underestimated because of the reason mentioned above. Similarly, values of Ω obtained from FAC are also comparable with those from the DARC and CB codes for many transitions, as also demonstrated by Aggarwal et al. [8–10]. However, for some transitions the values of Ω can be overestimated, both from DARC and FAC (see, for example, Fig. 4 of Aggarwal et al. [9]). This is because the CB approximation for elastic transitions is critically dependent on transition energy ΔE. As the degeneracy among the levels of a state of hydrogenic ions is very small, it is difficult to know the energy levels accurately. We discuss this point further in Sections 2.1 and 4.1.

2. Theory

2.1. CB approximation

The present treatment is non-relativistic, but the spin of atomic electron and the energy difference of fine-structure levels are taken into account. An atomic basis for partial wave J is defined by

$$\psi^J_{n\lambda jl}(\mathbf{x}, \sigma, \hat{r}) = R_{n\lambda}(x)\chi^J_{\lambda jl}(\hat{\mathbf{x}}, \sigma, \hat{r}) \quad (1)$$

where $R_{n\lambda}$ is the non-relativistic radial function of hydrogenic ion with nuclear charge Z, $\mathbf{x}(\mathbf{r})$ are the coordinates of atomic (incident) electron from the nucleus, $\sigma(\mathbf{s})$ is the spin variable (operator) of atomic electron, and $\chi^J_{\lambda jl}$ is a simultaneous eigenfunction of angular momentum operators $\mathbf{l}_x^2$, $\mathbf{s}^2$, $(\mathbf{l}_x + \mathbf{s})^2$, $\mathbf{l}_r^2$, and $\mathbf{J}^2 = (\mathbf{l}_x + \mathbf{s} + \mathbf{l}_r)^2$ with corresponding eigenvalues $\lambda(\lambda+1)$, $3/4$, $j(j+1)$, $l(l+1)$, and $J(J+1)$, respectively.