CALCULATION OF OSCILLATOR STRENGTH FOR SOME ATOMIC SERIES

THESIS

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By

MAGDY ALY ATTIA MOHAMED EL-SHOURA

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Thesis advisor

Prof. Ali H. Moussa

Dr. Gaber T. Omar

Dr. Hassan H. Ramadan

Approval

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( )

( )

Prof. M. A. El-Sharkawy

(Sharkawy)

Head of Physics Department

Faculty of Science

Ain Shams University

بسم الله الرحمن الرحيم

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Abstract

The radiative rates (A_r's), radiative life times (τ) and oscillator strengths (f-values) are calculated in AMA scheme for B-like Ne^{5+}, Al^{8+}, P^{10+}, Ar^{13+} and Sc^{16+} ions. All bound-state wave functions needed in these calculations are generated using Hartree-Fock (SCHF) program.
The trends of A_r's, τ's and f-values with atomic number (Z), effective charges (Z_{eff}) and principal quantum numbers n' (of upper levels) and n (of lower levels) are investigated. The f-values in AMA scheme are found in good agreement with that calculated in LS-coupling and MCFC (by others) for highly ionized ions.

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SUMMARY

Summary

The thesis deals with the study of oscillator strengths (f-values) for B-like ions. These f-values are interrelated with the radiative transition probabilities (A_r's) and life times (τ) of excited states. Thus, the f-values, A_r's and τ's are calculated for B-like Ne^{5+}, Al^{8+}, P^{10+}, Ar^{13+} and Sc^{16+}. Specifically, the emissive groups of transitions n's $\rightarrow$ np, n'd $\rightarrow$ np, n'p $\rightarrow$ ns and n'p $\rightarrow$ nd with $n \leq n'$; n' = 9,8,...,3 are involved in these calculations in details. The angular momentum average scheme (AMA) is utilized for all the calculations of f-values, A_r's and τ's. All bound state wave functions needed are generated using the single-configuration Hartree-Fock (SCHF) program (Froese Fischer code). The A_r's for highly ionized ions are also calculated using the hydrogenic program and compared with their corresponding values which are calculated using SCHF.

The trends of f-values, A_r's and τ's with the atomic number (Z), effective charge (Z_{eff}) and principal quantum numbers (n', n) of upper and lower states included in the transitions are investigated. The results in this thesis may be summarized in the following points:

1- A_r for certain Δn transitions with $\Delta \ell = +1$ are 6 times larger than that with $\Delta \ell = -1$ for Ne^{5+}. This ratio reaches 8 to 10 times for $Ar^{13+}$and Sc^{16+}.

2- A_r decreases rapidly with n' (of upper levels). Specifically, $A_r \sim \; / n'^3$. The variation of A_r with n' is smooth. However, the variation of A_r with n (of lower level) is found to be of irregular behavior.

3- A_r increases as Z_{eff}^4 for the B-isoelectronic series. Z_{eff}, here, is taken as $(Z_I + Z_C)/2$. where Z_I is the degree of ionization and Z_C is the atomic number respectively.

4- The calculated A_r^{HF} from Hartree-Fock is approximately equal to A_r^{HP} calculated using the hydrogenic program with $Z_{eff} = \sqrt{Z_I Z_C}$ for O^{3+}, and $Z_{eff} = (Z_I + Z_C)/2$ for Ne^{5+} up to Sc^{16+}.

5- The radiative life times vary as $1/Z^{4.5}$. For example, the excited state 6s has $\tau = 1.8 \times 10^{-10}$ sec in Ne^{5+} case and decreases to $\tau = 4.33 \times 10^{-12}$ sec in case of Sc^{16+}. In addition, τ varies as $(n')^{2.5}$ where n' is the principal quantum number of upper levels.

6- f-values are found large for n'd $\rightarrow$ 2p and the n'p $\rightarrow$ 3s transitions. The transition 3d $\rightarrow$ 2p has the largest f-values for B-like ions. f(3d $\rightarrow$ 2p) is equal to 0.427, 0.506, 0.538, 0.570 and 0.591 for Ne^{5+}, Al^{8+}, P^{10+}, Ar^{13+} and Sc^{16+} respectively.

7- f-values increase slowly with the atomic number (Z) i.e., decrease with 1/Z. However, these f-values are roughly independent of the effective charge (Z_{eff}), i.e. $f \sim Z_{eff}^0$.

8- f-values decrease as $1/n'^{4.5}$, where n' is the principal quantum number of upper level while these f-values increase with n which is the principal quantum number of lower level. The variation of f-values for 8d $\rightarrow$ np transitions with n contains an accidental cancellation in case of Ne^{5+}. This integral cancellation reduces the f-value at n = 6 by a factor of 10 . Such cancellation does not appear for P^{10+}, Ar^{13+} and Sc^{16+} at any value of n.

9- The f-values in the present work are found in good agreement with that of other theoretical calculations which are done in different coupling schemes for some available transitions. These transitions are $3s \rightarrow 2p$ and $3p \rightarrow 3s$ in both O^{3+} and Ne^{5+} cases as well as $3s \rightarrow 2p$, $4s \rightarrow 2p$ and $4s \rightarrow 3p$ in Al^{8+} case. Presumably, as the degree of ionization increases the f-values in different methods are approximately equal. Thus, for quantitative study of f-values for other atomic series needed in plasma modeling, AMA is good enough to be used.

CHAPTER I

Chapter I

Introduction

Recently, it is well-known that knowledge of oscillator strengths is needed in astrophysical and laboratory plasmas as well as laser physics.

Oscillator strength has relationships with the atomic transition probabilities (Einstein-coefficients) which are playing an important role in laser research .

Oscillator strength is of special interest in atomic and molecular spectroscopy since it is related to radiative width and radiative life times of excited states as well as line strength and intensity of spectral lines.

Oscillator strength is of great interest also in atomic collisions. It is utilized in the calculations of the cross sections of atomic processes which are taking place in hot plasmas such as dielectronic recombination (Burgess, 1964, 1965), photo- Auger ionization (Lagattuta and Hahn 1982, Jayanti and Steven, 1986) and photo-excitation. These processes are important in self cooling and ionization balance in hot laboratory plasma and in solar corona.

Oscillator strength is required in testing the accuracy of wave functions in the transitions under considerations.

Because of the above reasons, there is a growing interest in the study of oscillator strengths especially for ions (Guet G. 1990, Fawcett B. 1991, Tiwary S. 1991 a, b, 1993, Zilitis V. 1992 and Hibbert A. 1993) since they are dominantly included in atomic collisions and may lead to the production of X-ray or lasers.

Oscillator strength is a dimensionless quantity which has been introduced before the advent of the quantum theory (Geoffery V., 1968) and used to denote the distribution of an atom or molecule to absorb or to emit radiation from a certain state. Its physical meaning can be understood through the fact that the polarizability (dipole moment induced by an electric field strength) of the atom is equal to the sum of polarizabilities of atomic oscillators in which each oscillator is represented with strength (f-value).

In the present work, it was planned to calculate radiative (emissive) oscillator strengths for the B-isoelectronic sequence. The calculation of oscillator strengths (f-values), radiative transition probabilities (A_r's) and radiative life times (τ) depend mainly on the transition energy (ΔE) and the dipole matrix element (T).

All energies and wave functions needed in ΔE and T are generated using single-configuration Hartree-Fock (SCHF) program (Fischer code, 1977). These wave functions are employed in the matrix (MAT) program to calculate T and, in turn, gives out the radiative rates (A_r's). Both SCHF and