YU ISSN 0015—3206
FZKAAA 22 (4) 577 (1990)

OSCILLATOR STRENGTHS OF THE RESONANCE TRANSITION IN THE Rb I, Sr II, Cs I AND Ba II SYSTEMS

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Received 14 September 1990

UDC 539.19

Original scientific paper

We present relativistic calculations of the oscillator strengths for the resonance excitation $5p^6 5s\ ^2S^e \rightarrow 5p^6 5p\ ^2P^0$ transition in the Rb I and Sr II as well as $6p^6 6s\ ^2S^e \rightarrow 6p^6 6p\ ^2P^0$ transition in the Cs I and Ba II systems. Our present theoretical results are in good agreement with the available experimental data.

1. Introduction

Knowledge of both the length (f_L) and velocity (f_V) forms of the optical oscillator strengths is needed in astrophysics, plasma physics, atmospheric physics, laser physics and fusion research; it is also required in testing the accuracy of the wave functions involved in the transitions under consideration. The agreement between f_L and f_V indicates the accuracy of the wave functions. Accurate wave functions are needed for the reliable study of collision processes in atoms, molecules and ions.

It is well known that the use of relativistic quantum theory to treat problems in atomic and molecular physics has become common place in the last few years because standard computer packages developed by Desclaux[1], Hibbert[2], Glass and Hibbert[3], Grant et al.[4] and Dyall et al.[5] are generally available.

* A part of this work was done while the author was Research Director and Professor, CNRS Laboratory, University of Paris-Sud, Paris and Observatoire de Paris, Meudon, Paris, France.

Tiwary and his co-workers[6-22] have extensively investigated the excitation energies and oscillator strengths for different types of transitions in several atoms and ions. Our investigation shows that the inclusion of the effects of correlation and relativity is indispensable in obtaining reliable results in heavy alkali- metal atoms and ions.

In continuation of our earlier work on the inner-shell excitation energies and oscillator strengths, we extend our calculations to the rubidium and cesium isoelectronic sequences in exactly the same way as we did earlier in order to see the effect of the relativity on the excitation energies and oscillator strengths for the resonance excitation $5p^6 5s\ ^2S^e \rightarrow 5p^6 5p\ ^2P^0$ transition in the Rb I and Sr II as well as $6p^6 6s\ ^2S^e \rightarrow 6p^6 6p\ ^2P^0$ transition in the Cs I and Ba II systems.

2. *Method*

We have performed our relativistic calculations using the general configuration-interaction (CI) code CIV3 of Hibbert[2] and Glass and Hibbert[3]. The LS wave functions are written in the form

$$\Psi(LS) = \sum_{i=1}^{M} a_i \Phi_i (a_i LS). \tag{1}$$

The coefficients a_i are the eigenvectors components of the Hamiltonian matrix with typical element

$$H_{ij} = \langle \Phi_i | H | \Phi_j \rangle. \tag{2}$$

Φ_j are single-configuration functions constructed from one-electron functions, whose orbital and spin momenta are coupled to form the common total angular-momentum quantum numbers L and S according to a prescription denoted in (1) by a_i.

We express the radial parts of the one-electron functions in analytical form as a sum of Slater-type orbitals, following Clementi and Roetti[23]:

$$P_{nl} = \sum_{j=1}^{k} C_{jnl} r^{I_{jnl}} e^{-\xi_{jnl} r}. \tag{3}$$

The parameters in Eq. (3) can be varied to optimize the energy of any state, subject to the orthonormality conditions

$$\int_0^\infty P_{nl}(r)\, P_{n'l}(r)\, dr = \delta_{nn'}. \tag{4}$$

Once the radial wave functions are determined, relativistic effects may be added to the Hamiltonian in the form of the Breit-Pauli interaction, of which we include the spin-orbit, spin-other-spin, spin-spin, mass correction and one-body Darwin

terms. The first three terms split LS states into J-dependent levels while the last two affect the overall energy of each term. The expansion (1) is then replaced by

$$\Psi(J) = \sum_i a_i \Phi_i (LSJ) \tag{5}$$

where the summation now includes single-configuration with different L and S (which can couple to form a common J value). The matrix which is diagonalized to give the eigenenergies and eigenvectors components a_i now contain the Breit-Pauli operators as well as the previous non-relativistic terms in the Hamiltonian.

3. *Results and discussion*

Table 1 displays the relativistic excitation energies (ΔE in atomic unit) and oscillator strengths (f) for the resonance excitation $5p^6 5s\ ^2S^e \rightarrow 5p^6 5p\ ^2P^0$ transition in the Rb I and Sr II as well as $6p^6 6s^2 S^e \rightarrow 6p^6 6p\ ^2P^0$ transition in the Cs I and Ba II systems along with the available experimental results taken from the critical compilation for the alkali-metal atoms and their isoelectronic sequences by Martin and Wiese[24].

TABLE 1.

Systems	Our present results		Experimental results	
	ΔE	f	ΔE	f
Rb I	0.04881	0.3740	0.057	0.335
	0.04942	0.75507	0.058	0.675
Sr II	0.09913	0.39819	0.108	0.340
	0.10152	0.81337	0.112	0.710
Cs I	0.04231	0.38809	0.051	0.362
	0.04493	0.79907	0.053	0.732
Ba II	0.07891	0.42319	0.092	0.350
	0.08341	0.91907	0.100	0.740

Excitation energies and oscillator strengths of the resonance excitation $5p^6 5s\ ^2S^e \rightarrow 5p^6 5p\ ^2P^0$ transition in the Rb I and Sr II as well as $6p^6 6s\ ^2S^e \rightarrow 6p^6 6p\ ^2P^0$ transition in the Cs I and Ba II systems.

Several features of importance emerge from Table 1. First, it is clear from Table 1 that our theoretical excitation energy is smaller than the experimental value of the excitation energy in all systems of our present consideration. Second, the value of the oscillator strengths for the resonance transition in Sr II is larger than the value of the oscillator strength for Rb I which supports the experimental observations. Similar situation exists for the resonance transition in the Cs I and Ba II. Third, the value of the oscillator strength for the transition $\Delta J = 1$ is larger than the value of the oscillator strength for the transition $\Delta J = 0$ by about a factor of two in all systems of present consideration which agrees with the ex-

periment. Finally, the examination of Table 1 shows that our theoretical trend of the excitation energy as well as the oscillator strength agrees well with the experimental trend.

4. Conclusion

In general, the agreement is good between our present theoretical predictions and experimental observations which indicates the present results may be considered to be reliable. We hope that this work will stimulate other theoretical as well as experimental investigations.

Acknowledgements

The author would like to thank Professor Abdus Salam, the International Atomic Energy Agency and UNESCO, for hospitality at the International Center for Theoretical Physics, Trieste, Italy, and Swedish Agency for Research Cooperation with Developing Countries (SAREC) for financing my current Associateship visit. He is also grateful to Profs. Dujardin, Hellner, Le Rouzo, Gaillard (Director), Remy (Adj. Director) and Hibbert for encouragement and suggestions. Finally he wishes to express his thanks to Bihar University, India, for leave.

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OSCILACIJSKE JAKOSTI ZA REZONANCIJSKE PRIJELAZE U RgI, SrII, CsII i BaII SUSTAVIMA

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UDK 539.19

Originalni znanstveni rad

Relativistički računi oscilacijskih jakosti za rezonancijski prijelaz $5p^6 5s^2 S^e \rightarrow 5p^6 5p^2 P^0$ su dani za RbI i SrII te za prijelaz $6p^6 6s^2 S^e \rightarrow 6p^6 6p^2 S^0$ za CsI i Ba II. Teorijski su rezultati u dobrom slaganju s dostupnim eksperimentalnim podacima.