ABSOLUTE AND RELATIVE THEORETICAL VALUES OF OSCILLATOR STRENGTHS FOR CERTAIN LINES IN THE SiII AND GeII SPECTRA

By M. D. Kunisz and J. Migdałek

Laboratory of Atomic Optics, Institute of Physics, Jagellonian University, Cracow*

(Received February 17, 1973)

Relative and absolute values of spectral line strengths and oscillator strengths are calculated for certain transitions of the principal and sharp series in the ion spectra of SiII and GeII. Radial wave functions, obtained by the method of linear deformation of the ion core, were used. This method has been described in detail in earlier papers.

1. Introduction

In earlier papers [7], [8] a calculation was performed of absolute and relative values of line strengths and oscillator strengths in the AlI, GaI and InI atomic spectra. The problem encountered at that stage was the fact that a basic divergence between theoretical [5] and experimental [9], [10] ratios of line strengths was found for the sharp series. In papers [7] and [8] theoretical results were found to agree to within 30% with experimental results for those doublets for which experimental data exist. In the mentioned papers the obtained values were compared with theoretical and experimental data found in other papers on this subject.

In the present paper results are given of a calculation of absolute and relative values of radial transition integrals from which, in turn, corresponding values of spectral line strengths and oscillator strengths are calculated for certain transitions in the SiII and GeII spectra. Of particular interest is the Ge^+ ion for which no earlier values of relative and absolute oscillator strengths were found to be determined, neither theoretically nor experimentally. Calculations for the Si^+ ion, for which f_{ik} values were published for some transitions, are at the same time treated as a test of correctness of the method.

* Address: Zakład Optyki Atomowej, Instytut Fizyki UJ, Reymonta 4, 30-059 Kraków, Poland.

2. Calculations

Calculations were performed for the doublets of the principal series ($4p\,^2P^0_{1/2,\,3/2} \rightarrow 4s\,^2S_{1/2}$) $\lambda\lambda$ 6347.103, 6371.359 Å in SiII and ($5p\,^2P^0_{1/2,\,3/2} \rightarrow 5s^2S_{1/2}$) $\lambda\lambda$ 5895.01, 6022.67 Å in GeII as well as for doublets of the sharp series $ns\,^2S_{1/2} \rightarrow 3p\,^2P^0_{1/2,\,3/2}$ and $ms\,^2S_{1/2} \rightarrow 4p\,^2P^0_{1/2,\,3/2}$ for SiII and $n's\,^2S_{1/2} \rightarrow 4p\,^2P^0_{1/2,\,3/2}$ and $m's\,^2S_{1/2} \rightarrow 5p\,^2P^0_{1/2,\,3/2}$ for GeII.

Absolute values of line strengths were evaluated [1] from the following formula in atomic units:

$$S(nlj;\, n'l'j') = 2Q(\tfrac{1}{2}\, lj;\, \tfrac{1}{2}\, l'j')\, l_{\max} \chi^{n'l'j'}_{nlj}$$

where: $l_{\max} = \max(l, l')$

$$Q(\tfrac{1}{2}\, lj;\, \tfrac{1}{2}\, l'j') = \tfrac{1}{2}(2j+1)(2j'+1) W^2(ljl'j';\, \tfrac{1}{2}\, 1),$$

W is the Racah coefficient,

$$\chi^{n'l'j'}_{nlj} = \int_0^\infty P_{n'l'j'}(r) P_{nlj}(r) r dr,$$

and oscillator strengths, f_{ik}, from the formula:

$$f_{ik} = \frac{3.04 \cdot 10^2}{g_i \lambda} S_{ki}$$

where i is the lower state, and k the higher one, g_i is the statistical weight of the lower state, λ, wavelength in angstrems and S_{ki} line strength in atomic units.

The function $P_{nlj}(r)$ is connected with the radial part $R_{nlj}(r)$ of the wave function of the optical electron $\psi_{nlj}(r)$ describing its state [2], taking into account the coupling between its orbital momentum l and its spin s, by the formula:

$$R_{nlj}(r) = \frac{P_{nlj}(r)}{r}.$$

One obtains this function for $l \neq 0$ by the use of the first-order perturbation theory [3]. Taking the interaction Hamiltonian [4] to be of the shape

$$H' = \frac{1}{4 \cdot (137)^2} \frac{1}{r} \frac{dV}{dr} \vec{L} \cdot \vec{\sigma}$$

we obtain [5]:

$$P_{nlj}(r) = P_{nl}(r) + \begin{Bmatrix} l \\ -l(l+1) \end{Bmatrix} \frac{1}{4 \cdot (137)^2} \sum_{n' \neq n} \frac{\int_0^\infty P_{nl}(r) \frac{1}{r} \frac{dV}{dr} P_{n'l}(r) dr}{E^{(0)}_{nl} - E^{(0)}_{n'l}} P_{n'l}(r)$$

for

$$j = \begin{cases} l+1/2 \\ l-1/2 \end{cases} \text{ respectively; } V(r) = -\frac{\zeta(r)}{r}$$

where $\zeta(r)$ is the effective charge of the field in which the optical electron is present.

The P_{nl} functions which correspond to the terms were obtained by the semi-empirical method of linear deformation of the ion core (or atom core), proposed by Weinstein [6]. The function P_{nl} is in this case the solution of the following equation:

$$\frac{d^2P_{nl}(r)}{dr^2} + \left\{ \frac{2\zeta\left(\frac{r}{\omega}\right)}{r} - \frac{l(l+1)}{r^2} - 2\varepsilon \right\} P_{nl}(r) = 0$$

where $\zeta\left(\frac{r}{\omega}\right)$ is the effective charge of the ion core field and ε the experimental value of ionisation energy of the optical electron in the state described by the function P_{nl} (taken from appropriate tables [11]). ω is the parameter of linear deformation of the ion core.

The above equation was solved numerically and the parameter ω was chosen in such a way as to obtain n-l–1 nods for the P_{nl} function. For large r the following asymptotical solution was used:

$$P_{nl}(r) = Ar^{\mu}e^{-\alpha r}$$

where: A is the normalizing constant, $\mu = \frac{Z-N}{\alpha}$, N is the number of electrons in the atom core and $\alpha = \sqrt{2\varepsilon}$.

More detailed remarks concerning the calculations may be found in earlier papers [7] and [8].

All calculations were performed by a single program prepared for the ODRA 1204 computer.

3. *Results and conclusions*

For both ions, Si^+ and Ge^+, a weak dependence of the ion core deformation parameter on the principal quantum number n at a fixed orbital quantum number l, was found. For Si^+ ω behaves unmonotonically with variation of n and it is contained within the range of values $\langle 1.173–1.232\rangle$, for s-states, and within the range $\langle 1.128–1.174\rangle$ for p-states. Correspondingly, for s-states in Ge^+ we find the range to be $\langle 1.115–1.141\rangle$, and $\langle 1.085–1.105\rangle$ for p-states. The dependence of ω on n is thus stronger for Si^+ than that for Ge^+. It should be noted that also for the Al-group this dependence was weak, which, according to [6] guarantees the approximate orthogonality of wave functions P_{nl} for different n.

TABLE I

Si II

Transition	S_2/S_1
Principal series	
$4p^2P^0_{3/2,1/2} - 4s^2S_{1/2}$	1.998
Sharp series	
$4s^2S_{1/2} - 3p^2P^0_{3/2,1/2}$	2.031
$5s^2S_{1/2} - 3p^2P^0_{3/2,1/2}$	2.035
$6s^2S_{1/2} - 3p^2P^0_{3/2,1/2}$	2.049
$7s^2S_{1/2} - 3p^2P^0_{3/2,1/2}$	1.917
$5s^2S_{1/2} - 4p^2P^0_{3/2,1/2}$	2.023
$6s^2S_{1/2} - 4p^2P^0_{3/2,1/2}$	2.021
$7s^2S_{1/2} - 4p^2P^0_{3/2,1/2}$	1.962

TABLE II

Ge II

Transition	S_2/S_1
Principal series	
$5p^2P^0_{3/2,1/2} - 5s^2S_{1/2}$	1.987
Sharp series	
$5s^2S_{1/2} - 4p^2P^0_{3/2,1/2}$	2.136
$6s^2S_{1/2} - 4p^2P^0_{3/2,1/2}$	2.114
$7s^2S_{1/2} - 4p^2P^0_{3/2,1/2}$	2.137
$8s^2S_{1/2} - 4p^2P^0_{3/2,1/2}$	1.576
$9s^2S_{1/2} - 4p^2P^0_{3/2,3/2}$	1.517
$10s^2S_{1/2} - 4p^2P^0_{3/2,1/2}$	1.490
$6s^2S_{1/2} - 5p^2P^0_{3/2,1/2}$	2.101
$7s^2S_{1/2} - 5p^2P^0_{3/2,1/2}$	2.058
$8s^2S_{1/2} - 5p^2P^0_{3/2,1/2}$	1.777
$9s^2S_{1/2} - 5p^2P^0_{3/2,1/2}$	1.728
$10s^2S_{1/2} - 5p^2P^0_{3/2,1/2}$	1.702

In Table I values of ratios of line strengths for calculated SiII transitions are presented. Similar quantities are presented for GeII in Table II. In Figs 1 and 2 the dependence is plotted of line strength ratios on the n value of the upper state in the sharp series of SiII and GeII, as compared with similar dependences for AlI and GaI respectively, as taken from [8].

From the above tables and plots it follows that for transitions in the sharp series to $3p$ in SiII as well as for doublets with the lower state $4p$ in GeII, this dependence is non-

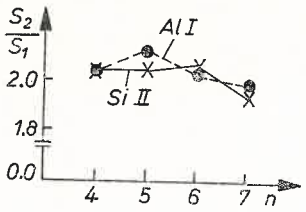

Fig. 1. SiII

monotonic. However, relative line strengths for the series of transitions ending with the state $4p$ in SiII, as well as for those ending with the state $5p$ in GeII, diminish with increasing value of the principal quantum number. One should note that strength ratios for lines GeII $ms \rightarrow 5p$ for $m = 8, 9, 10$ have an especially low value. In Tables III and IV

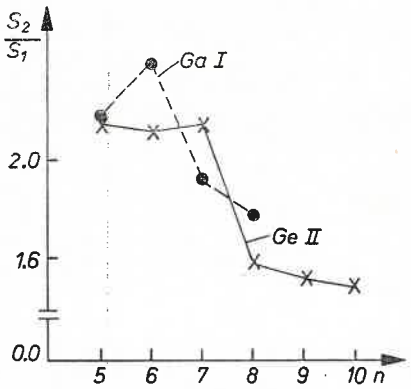

Fig. 2. GeII

are presented absolute values of oscillator strengths for some calculated transitions in the GeII and SiII spectra. In all cases with the exception of the transition $7s\ ^2S \rightarrow 3p\ ^2P^0$ in GeII, these values diminish rapidly with the increase of the principal quantum number n of the upper state, within a given series.

In Tables V, VI and VII a comparison is made between values $g_i f_{ik}$ (g_i being the weight of the upper state and f_{ik} the oscillator strength for an absorption transition) for certain

transitions in the Si^+ ion, and values taken from other experimental and theoretical data. Moreover, in Table VII, the obtained value of the transition probability for the transition $4s\ ^2S \rightarrow 3p\ ^2P^0$ in SiII is compared with the corresponding value taken from another paper [18]. In all cases for which data exist, good agreement is found between values

TABLE III

Si II

Transition	$J-J'$	f_{ik}
Principal series		
$4p^2P^0 - 4s^2S$	3/2–1/2 1/2–1/2	0.856 0.427
Sharp series		
$4s^2S - 3p^2P^0$	1/2–3/2 1/2–1/2	0.114 0.113
$5s^2S - 3p^2P^0$	1/2–3/2 1/2–1/2	0.016 0.016
$6s^2S - 3p^2P^0$	1/2–3/2 1/2–1/2	0.0073 0.0071
$7s^2S - 3p^2P^0$	1/2–3/2 1/2–1/2	0.0097 0.0101
$5s^2S - 4p^2P^0$	1/2–3/2 1/2–1/2	0.229 0.227
$6s^2S - 4p^2P^0$	1/2–3/2 1/2–1/2	0.0329 0.0327
$7s^2S - 4p^2P^0$	1/2–3/2	0.0289

of f_{ik} or A_{ki} obtained in this paper and those taken from other theoretical and experimental works.

As may be seen from Tables I and II, relative values of line strengths in the sharp series of SiII and GeII spectra for the first doublets usually increase slightly with increasing doublet number and for further ones diminish at first slightly and then more rapidly only for transitions from very high s-states (see remark concerning GeII). They remain, however, within range $1.962 \leqslant \frac{S_2}{S_1} \leqslant 2.049$ for SiII and $1.490 \leqslant \frac{S_2}{S_1} \leqslant 2.137$ for GeII.

TABLE IV

Ge II

Transition	$J - J'$	f_{ik}
Principal series		
$5p^2P^0 - 5s^2S$	3/2–1/2 1/2–1/2	0.917 0.451
Sharp series		
$5s^2S - 4p^2P^0$	1/2–3/2 1/2–1/2	0.137 0.132
$6s^2S - 4p^2P^0$	1/2–3/2 1/2–1/2	0.0183 0.0177
$6s^2S - 5p^2P^0$	1/2–3/2 1/2–1/2	0.257 0.251
$8s^2S - 5p^2P^0$	1/2–3/2 1/2–1/2	0.0276 0.0313
$9s^2S - 5p^2P^0$	1/2–3/2 1/2–1/2	0.0199 0.0232

TABLE V

Si II

Transition \ Paper	$g_i f_{ik}$ Theor. [12]	Theor. [13]	Exper. [14]	Theor. [15]	Exper. [16]	Exper. [17]	Theor. Present paper
$4s^2S_{1/2} - 4p^2P^0_{3/2}$	1.901	1.640	1.78	1.77	—	1.51	1.712
$4s^2S_{1/2} - 4p^2P^0_{1/2}$	0.947	0.818	0.89	0.88	0.86	0.86	0.854

TABLE VI

Si II

Transition \ Paper	$g_i f_{ik}$ Theor. [12]	Theor. [13]	Exper. [14]	Exper. [16]	Exper. [17]	Theor. [15]	Theor. Present paper
$4p^2P^0_{3/2} - 5s^2S_{1/2}$	1.039	0.860	0.60	0.605	1.01	—	0.916
$4p^2P^0_{1/2} - 5s^2S_{1/2}$	0.522	0.424	0.30	—	0.50	—	0.454

TABLE VII

Si II

Probab. of transition \ Paper	Theor. [15]	Exper. [18]	Exper. [19]	Theor. Present paper
$A_{4s^2S-3p^2P^0}$ $(10^{-8}s^{-1})$	—	11.1	—	9.7
$f_{3p^2P^0-4s^2S}$	0.13	—	0.086	0.11

The above results, on comparison with corresponding values obtained for the spectra of other Al-like atoms, seem reasonable, however a more thorough opinion will be possible only after the completion of measurements which are currently under way in the Laboratory of Atomic Optics.

REFERENCES

[1] J. J. Sobelman, *Vvedenie v teoriu atomnykh spektrov*, GIFFL, Moskva 1963.
[2] W. Hartree, D. Hartree, *The Calculation of Atomic Structure*, John Wiley Sons, New York 1957.
[3] B. Średniawa, *Mechanika kwantowa*, PWN, Warszawa 1970, in Polish.
[4] E. Fermi, *Z. Phys.*, **59**, 680 (1930).
[5] W. Hanus, *Bull. Acad. Polon. Sci., Ser. Sci. Math. Astron. Phys.*, **8**, 629 (1960).
[6] L. A. Weinstein, *Trudy FIAN*, **15**, 3 (1961).
[7] M. D. Kunisz, J. Dobrzańska, J. Migdałek (to be published).
[8] J. Migdałek, *Zeszyty Naukowe UJ* (in press).
[9] M. D. Kunisz, *Acta Phys. Polon.*, **17**, 455 (1957).
[10] N. P. Penkin, L. N. Shabanowa, *Optika i Spektrosk.*, **14**, 1, 12, 167 (1963).
[11] Ch. Moore, *Atomic Energy Levels*, National Bureau of Standards, USA, 1958.
[12] Ch. Froese, A. B. Underhill, *Astrophys. J.*, **146**, 301 (1966).
[13] H. R. Griem, *NRL Rept.* No 6084 (1964).
[14] H. G. Groth, *Z. Astrophys.*, **51**, 231 (1960).
[15] L. Biermann, K. Lubeck, *Z. Astrophys.*, **25**, 325 (1948).
[16] P. Hey, *Z. Phys.*, **157**, 79 (1959).
[17] E. Shulz-Gulde, *J. Quant. Spectrosc. Radiative Transfer*, **9**, 113 (1969).
[18] J. Savage, *Astrophys. J.*, **146**, 940 (1966).
[19] W. Hoffmann, *Z. Naturforsch.*, **24a**, 6 (1969).