

OSCILLATOR STRENGTHS FOR S VI, Cl VII, Ar VIII AND K IX

S. N. TIWARY*, D. D. SINGH and P. KUMAR

International Centre for Theoretical Physics, Trieste, Italy

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The oscillator strengths, of both the length and velocity forms, for the inner-shell excitation $1s^2 2s^2 2p^6 3s^2 S^e \rightarrow 1s^2 2s^2 2p^5 3s^2 {}^2P^o$ transition, which leads to auto-ionization (Auger transition), in S VI, Cl VII, Ar VIII and K IX ions of the sodium isoelectronic sequence have been calculated using the approach suggested by one of us (S. N. Tiwary) in the case of P V ion. Our present calculated results demonstrate that the Tiwary approach is capable of yielding encouraging results.

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.

There is a growing interest in the study of ionized atoms because they are of astrophysical interest; for example, the spectra of quasi-stellar objects are now generally interpreted as a red-shifted absorption and emission lines of ionized atoms¹⁾. The electric dipole oscillator strengths of these ions are of intense inte-

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

rest for the diagnostics of both natural and astrophysical plasmas. Study of the inner-shell excitation of atoms and ions has also been of considerable interest for both experimentalists and theorists, because inner-shell excitation, in general, leads to autoionization, which plays a very important role in explaining the structure observed in the total ionization cross section curve for electron impact.

Consequently, much of current theoretical as well as experimental work is devoted to evaluate the accurate oscillator strengths of the inner-shell excitation process in atoms and ions. From theoretical point of view, accurate oscillator strengths can be expected only if accurate wave functions are employed in the transition matrix elements. If the wave functions are exact, the length and velocity forms of the oscillator strengths (f_L and f_V , respectively) will be equal.

Tiwary and his co-workers²⁻¹⁹⁾ have extensively investigated the length and velocity forms of the oscillator strengths using Hartree-Fock (HF) and configuration-interaction (CI) wave functions for different types of transitions in several atoms and ions. Very recently, Tiwary et al.¹⁶⁾ have calculated the HF and large CI oscillator strengths of several transitions in the sodium isoelectronic sequence. The inner-shell excitation of the P^{4+} ion has also been investigated. However, there is a large discrepancy between the CI f_L and f_V for the inner-shell excitation, which leads to autoionization, in the P^{4+} ion. Most recently, Tiwary¹⁹⁾ has shown that the discrepancy can be removed and an excellent agreement can be achieved between the CI f_L and f_V , if the condition $\langle r_{2p} \rangle \approx \langle r_{3p} \rangle \approx \langle r_{3d} \rangle$ is satisfied in the calculations.

The main goal this paper is to generalize the Tiwary approach and to extend the investigation to the ionized atoms of the sodium isoelectronic sequence where the effect of relativity is not very important and offers the best opportunity to test the utility of the Tiwary approach.

2. Method

We have performed our CI calculation using the computer program CIV3 of Hibbert²⁰⁾ in the same way as in our earlier work²⁻¹⁹⁾. The CI wave function is written as

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

Each of the M single-configuration functions Φ_i is 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 Eq. (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 Roetti²¹⁾:

$$P_{nl} = \sum_{j=1}^k C_{jnl} r^{l_{jnl}} e^{-\zeta_{jnl} r}. \quad (2)$$

The parameters in Eq. (2) can be varied to optimize the energy of any state, subject to the orthogonality conditions

$$\int_0^\infty P_{n'l}(r) P_{n'l'}(r) dr = \delta_{nn'}. \quad (3)$$

Once wave functions of form (1) have been determined in this way, they can be used to obtain the optical oscillator strengths, f_L and f_V , for transitions between initial and final states Ψ^i and Ψ^f , respectively:

$$f_L = \frac{2\Delta E}{3g_i} |\langle \Psi^i | \sum_{p=1}^N r_p | \Psi^f \rangle|^2 \quad (4)$$

and

$$f_V = \frac{2}{3g_i\Delta E} |\langle \Psi^i | \sum_{p=1}^N \nabla_p | \Psi^f \rangle|^2 \quad (5)$$

where $\Delta E = E^f - E^i$ and $g_i = (2L_i + 1)(2S_i + 1)$ is the statistical weight of the lower state Ψ^i . For the exact wave functions, Eqs. (4) and (5) give identical results. For approximate wave functions the two equations may yield different results. The reliability of either depends on the closeness of f_L and f_V . The parameters for the bound orbitals of the S VI, Cl VII, Ar VIII and K IX ions are given in Tables 1—4.

TABLE 1.

| Orbital | Coefficient | Power of r | Exponent |
|---------|---------------|--------------|------------|
| 1s | 119.821335 | 1 | 16.4963989 |
| | 4.6495500 | 1 | 25.5415039 |
| | 0.3611770 | 2 | 6.1169300 |
| | 103.2056580 | 2 | 14.8109999 |
| | 0.0009033 | 3 | 2.6577797 |
| 2s | -0.1074218 | 3 | 5.2086096 |
| | -32.4716949 | 1 | 16.4963989 |
| | -2.0730858 | 1 | 25.5415039 |
| | 102.1504520 | 2 | 6.1169300 |
| | -135.9703220 | 2 | 14.8109999 |
| 3s | -0.0058072 | 3 | 2.6577797 |
| | 22.4305472 | 3 | 5.2086096 |
| | 12.1821918 | 1 | 16.4963989 |
| | 0.3175446 | 1 | 25.5415039 |
| | -39.8619385 | 2 | 6.1169300 |
| 2p | 49.5702515 | 2 | 14.8109999 |
| | 15.0544815 | 3 | 2.6577797 |
| | -28.4477081 | 3 | 5.2086096 |
| | 41.6719360 | 2 | 4.8570004 |
| | 67.7556305 | 2 | 8.0011196 |
| 3p | 19.4120178 | 2 | 14.2140999 |
| | 262.3681640 | 2 | 4.8570004 |
| | -2668.1621100 | 3 | 8.0011196 |
| 3d | 106.4699860 | 3 | 4.8570004 |

Parameters for the bound orbitals used in the present calculation. Each orbital is a sum of Slater type orbitals.

TABLE 2.

| Orbital | Coefficient | Power of r | Exponent |
|---------|---------------|--------------|------------|
| 1s | 130.695892 | 1 | 17.2886963 |
| | 5.8263245 | 1 | 26.9951019 |
| | 0.5030889 | 2 | 6.5224705 |
| | 93.9735413 | 2 | 15.5808001 |
| | 0.0037214 | 3 | 2.9942503 |
| 2s | -0.2270774 | 3 | 5.5827303 |
| | -36.3567963 | 1 | 17.2886963 |
| | -2.1431303 | 1 | 26.9951019 |
| | 123.7515410 | 2 | 6.5224705 |
| | -153.3795780 | 2 | 15.5808001 |
| 3s | -0.0170398 | 3 | 2.9942503 |
| | 23.6678772 | 3 | 5.5827303 |
| | -14.3052683 | 1 | 17.2886963 |
| | -0.2861259 | 1 | 26.9951019 |
| | 50.6248932 | 2 | 6.5224705 |
| 2p | -58.4884796 | 2 | 15.5808001 |
| | -23.5447540 | 3 | 2.9942503 |
| | 40.8027496 | 3 | 5.5827303 |
| | 53.8704529 | 2 | 5.3515701 |
| | 79.0834503 | 2 | 8.6442900 |
| 3p | 22.1111145 | 2 | 15.3242998 |
| | 364.7158200 | 2 | 5.3515701 |
| 3d | -3820.6162100 | 3 | 8.6442900 |
| | 149.4937440 | 3 | 5.3515701 |

Parameters for the bound orbitals used in the present calculation. Each orbital is a sum of Slater-type orbitals.

3. Results and discussion

Tables 5—8 show the configurations used for the excited $2P^0$ state in the present calculation for the S VI, Cl VII, Ar VIII and K IX ions, respectively. The numbers below the configurations give their weights. Table 9 displays the Hartree-Fock (HF) and configuration-interaction (CI) optical oscillator strengths, of both the length and velocity forms (f_L and f_V), respectively, of the inner-shell excitation $1s^2 2s^2 2p^6 3s^2 S^e \rightarrow 1s^2 2s^2 2p^5 3s^2 2P^0$ transition, which leads to auto-ionization (Auger transition), in S VI, Cl VII, Ar VIII and K IX ions of the sodium isoelectronic sequence.

Several features of importance emerge from Table 9. First, we notice that the HF f_L and f_V differ substantially with each other. This indicates that the HF description is not adequate for the accurate determination of the oscillator strengths for the complex inner-shell excitation transition. There is an excellent agreement between our present CI f_L and f_V obtained employing the Tiwary approach. This reflects the validity of the Tiwary approach. Second, in our earlier large CI calculations¹⁶⁾ of the oscillator strengths for the inner-shell excitation transition in the P^{4+} ion, significant discrepancy exists. The possible reason for the substantial disagreement between f_L and f_V was speculated in our earlier paper¹⁶⁾ due to the neglect of the effect of the relativity. The present investigation indicates that

TABEL 3.

| Orbital | Coefficient | Power of r | Exponent |
|---------|---------------|--------------|------------|
| 1s | 107.906937 | 1 | 18.1484070 |
| | 4.9286451 | 1 | 28.2234955 |
| | 0.4062686 | 2 | 6.8971996 |
| | 82.4930267 | 2 | 16.2752075 |
| | 0.0015250 | 3 | 3.3372498 |
| 2s | -0.1374697 | 3 | 5.8264399 |
| | -40.7728389 | 1 | 18.1484070 |
| | -1.8142719 | 1 | 28.2234955 |
| | 148.1412350 | 2 | 6.8971996 |
| | -171.0704190 | 2 | 16.2752075 |
| 3s | -0.0452332 | 3 | 3.3372498 |
| | 19.7397919 | 3 | 5.8264399 |
| | -16.4043884 | 1 | 18.1484070 |
| | -0.3508571 | 1 | 28.2234955 |
| | 63.8096313 | 2 | 6.8971996 |
| 2p | -70.5056763 | 2 | 16.2752075 |
| | -35.7065125 | 3 | 3.3372498 |
| | 52.3969269 | 3 | 5.8264399 |
| | 67.8363647 | 2 | 5.8418102 |
| | 90.9672699 | 2 | 9.2710505 |
| 3p | 25.1875763 | 2 | 16.2095947 |
| | 492.7900390 | 2 | 5.8418102 |
| 3d | -5303.8007800 | 3 | 9.2710505 |
| | 203.1677860 | 3 | 5.8418102 |

Parameters for the bound orbitals used in the present calculation. Each orbital is a sum of Slater-type orbitals.

the effect of the relativity is not very important in order to achieve an excellent agreement but inclusion of correlation is indispensable in the way suggested by Tiwary. Third, it is clear from Table 9 that (i) the oscillator strengths decrease with increase of atomic number (Z) and (ii) the correlation enhances the values of the oscillator strengths in the all ions of present consideration. Finally, our experience of the extensive theoretical investigations of the oscillator strengths of the inner-shell excitation in atoms and ions shows that it is very difficult to obtain an excellent agreement between f_L and f_V even using a huge number of configurations. However, in this work we have for the first time obtained an excellent agreement between the CI length and velocity values.

4. Conclusions

Our present theoretical investigation demonstrates that the Tiwary approach is very compact, convenient and economic from the computational point of view as well as capable of yielding the encouraging results for the complex inner-shell

TABLE 4.

| Orbital | Coefficient | Power of r | Exponent |
|---------|---------------|--------------|------------|
| 1s | 154.777039 | 1 | 19.2205963 |
| | 6.9090109 | 1 | 29.5917969 |
| | 0.5685759 | 2 | 7.2913904 |
| | 105.1875310 | 2 | 17.2931976 |
| | 0.0088466 | 3 | 3.6774502 |
| 2s | -0.2954897 | 3 | 6.1571102 |
| | -44.4382935 | 1 | 19.2205963 |
| | -2.3920794 | 1 | 29.5917969 |
| | 174.3359370 | 2 | 7.2913904 |
| | -206.8572690 | 2 | 17.2931976 |
| 3s | -0.0474498 | 3 | 3.6774502 |
| | 17.6976776 | 3 | 6.1571102 |
| | -18.2905884 | 1 | 19.2205963 |
| | -0.6954063 | 1 | 29.5917969 |
| | 77.9046173 | 2 | 7.2913904 |
| 2p | -89.4486542 | 2 | 17.2931976 |
| | -51.7964172 | 3 | 3.6774502 |
| | 70.3678894 | 3 | 6.1571102 |
| | 83.9009857 | 2 | 6.3336000 |
| | 102.9573820 | 2 | 9.8823004 |
| 3p | 28.9891510 | 2 | 16.9450989 |
| | 654.1452640 | 2 | 6.3336000 |
| 3d | -7200.7695300 | 3 | 9.8823004 |
| | 269.5974120 | 3 | 6.3336000 |

Parameters for the bound orbitals used in the present calculation. Each orbital is a sum of Slater-type orbitals.

excitation transition, which leads to autoionization, in the ionized atoms of the sodium isoelectronic sequence. This approach may provide significant advantages also in the case of the CI calculations in molecules, clusters and solids. The present CI wave function may be of use for calculations of scattering cross sections for the Auger process in S VI, Cl VII, Ar VIII and K IX ions. We hope that this work will stimulate experimental as well as other theoretical investigations.

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TABLE 5.

| $2p^0$ | $2p^5 3p^2 (^3P)$ | $2p^5 3s (^3P) 3d$ | $2p^5 3p^2 (^1D)$ | $2p^5 3s (^1P) 3d$ | $2p^5 3s^2$ |
|--------------------|-------------------|--------------------|-------------------|--------------------|--------------|
| $2p^5 3s^2$ | 0.00000515 | 0.01555226 | -0.00000726 | -0.00197477 | 0.99987698 |
| $2p^5 3s (^1P) 3d$ | 0.00191656 | -0.49935657 | -0.00261167 | 0.86633879 | 0.00947807 |
| $2p^5 3s (^3P) 3d$ | -0.00350657 | -0.86624974 | 0.00478864 | -0.49941993 | 0.01248747 |
| $2p^5 3p^2 (^3P)$ | -0.79614532 | -0.00006454 | -0.60510635 | -0.00010009 | 0.00000051 |
| $2p^5 3p^2 (^1D)$ | -0.60509288 | 0.00352340 | 0.79612684 | 0.00576988 | -0.000003451 |

Configurations used for the excited $2p^0$ state in the present calculation. The numbers below the configuration give their weights.

TABLE 6.

| $2p^0$ | $2p^5 3p^2 (^3P)$ | $2p^5 3s (^3P) 3d$ | $2p^5 3p^2 (^1D)$ | $2p^5 3s (^1P) 3d$ | $2p^5 3s^2$ |
|--------------------|-------------------|--------------------|-------------------|--------------------|--------------|
| $2p^5 3s^2$ | 0.00000325 | -0.01611031 | 0.00000449 | -0.00271446 | 0.99986649 |
| $2p^5 3s (^1P) 3d$ | -0.00149081 | -0.50015128 | -0.00201027 | -0.86587173 | -0.01040932 |
| $2p^5 3s (^3P) 3d$ | 0.00269904 | -0.86578530 | 0.00364394 | 0.50023806 | -0.01259188 |
| $2p^5 3p^2 (^3P)$ | -0.79597998 | 0.00003457 | 0.60532355 | -0.00005485 | 0.00000028 |
| $2p^5 3p^2 (^1D)$ | -0.60531557 | -0.00267419 | -0.79596913 | 0.00443516 | -0.000002550 |

Configurations used for the excited $2p^0$ state in the present calculation. The numbers below the configurations give their weights.

TABLE 7.

| $2P^0$ | $2p^53p^2(^3P)$ | $2p^53s(^3P)3d$ | $2p^53p^2(^1D)$ | $2p^53s(^1P)3d$ | $2p^53s^2$ |
|-----------------|-----------------|-----------------|-----------------|-----------------|-------------|
| $2p^53s^2$ | 0.00000204 | -0.01646665 | 0.00000274 | -0.00327646 | 0.99985886 |
| $2p^53s(^1P)3d$ | -0.00115403 | -0.50083417 | -0.00152414 | -0.86547023 | -0.01108428 |
| $2p^53s(^3P)3d$ | 0.00207162 | -0.86538494 | 0.00273792 | 0.50093812 | -0.01261047 |
| $2p^53p^2(^3P)$ | -0.79199082 | 0.00001843 | 0.61053252 | -0.00002980 | 0.00000015 |
| $2p^53p^2(^1D)$ | 0.59045368 | -0.00161368 | -0.79198480 | 0.00337434 | -0.00001869 |

Configurations used for the excited $2P^0$ state in the present calculation. The numbers below the configurations give their weights.

TABLE 8.

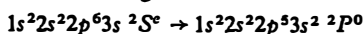
| $2P^0$ | $2p^53p^2(^3P)$ | $2p^53s(^3P)3d$ | $2p^53p^2(^1D)$ | $2p^53s(^1P)3d$ | $2p^53s^2$ |
|-----------------|-----------------|-----------------|-----------------|-----------------|-------------|
| $2p^53s^2$ | 0.00000123 | -0.01667833 | 0.00000164 | -0.00372746 | 0.99985409 |
| $2p^53s(^1P)3d$ | -0.00086254 | -0.50153750 | -0.00113842 | -0.86505753 | -0.01159097 |
| $2p^53s(^3P)3d$ | 0.00153782 | -0.86497372 | 0.00203044 | 0.50165355 | -0.01255826 |
| $2p^53p^2(^3P)$ | -0.79329228 | 0.00000963 | 0.60884124 | -0.00001584 | 0.00000008 |
| $2p^53p^2(^1D)$ | -0.60883904 | -0.00148683 | -0.79328829 | 0.00251324 | -0.00001338 |

Configurations used for the excited $2P^0$ state in the present calculation. The numbers below the configurations give their weights.

TABLE 9.

| Systems | functions | f_L | f_V |
|---------|-----------|-------|-------|
| S VI | HF | 0.076 | 0.068 |
| S VI | CI | 0.094 | 0.095 |
| Cl VII | HF | 0.075 | 0.068 |
| Cl VII | CI | 0.094 | 0.096 |
| Ar VIII | HF | 0.074 | 0.067 |
| Ar VIII | CI | 0.093 | 0.095 |
| K IX | HF | 0.072 | 0.066 |
| K IX | CI | 0.092 | 0.094 |

Optical oscillator strength of the inner-shell excitation



transition in S VI, Cl VII, Ar VIII and K IX ions of the sodium isoelectronic sequence.

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OSCILACIJSKE JAKOSTI ZA S VI, Cl VII, Ar VIII i K IX

S. N. TIWARY, D. D. SINGH i P. KAMUR

International Centre for Theoretical Physics, Trieste, Italy

UDK 539.19

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Oscilacijske jakosti, dužnih i brzinskih oblika, za pobuđenje u unutrašnjoj ljuski $1s^2 2s^2 2p^6 3s^2 S^e \rightarrow 1s^2 2s^2 2p^5 3s^2 P^0$ koje dovodi do autoionizacije (Auger prijelaz) u S VI, Cl VII, Ar VIII i K IX iona, računani su metodom predloženom S. N. Tiwary-a za slučaj PV iona. Teorijski rezultati pokazuju da je metodom Tiwary-a moguće postići ohrabrujuće rezultate.