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# Sternheimer valence shielding and antishielding factors for several 2p and 3p atoms and ions

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The Sternheimer valence shielding and antishielding factor $R$ has been calculated for the isoelectronic series of atoms in $2p^1$, $2p^2$, $2p^4$, $2p^5$, $3p^1$, $3p^4$, and $3p^5$ electronic configurations by means of the uncoupled numerical Hartree-Fock method. A slightly larger shielding effect is observed for the $^1D$ state relative to the $^3P$ state for $N^-$, O, and S. In the $2p^4$ series, where $N^-$ is included, it is found that the mononegative ion is characterized by an $R$ which is twice as large as that for the isoelectronic neutral atom. The general trends observed in the variation of $R$ within an isoelectronic series are discussed.

## I. INTRODUCTION

Experimental methods such as optical pumping, beam-foil technique, and nuclear quantum beats provide new possibilities of measuring the hyperfine interaction in the free ionic states. The measured quadrupolar interaction can be used to obtain the nuclear quadrupole moment $Q$ according to

$$Q = Q_{\text{expt}}(1-R)^{-1}, \tag{1}$$

where $Q_{\text{expt}}$ denotes the experimental estimate of the nuclear quadrupole moment uncorrected for the quadrupolar polarization induced in the core electrons which is accounted for in terms of the Sternheimer valence shielding factor[1] $R$. The purpose of this paper is to report the results of our calculations of $R$ using analytic Hartree-Fock (HR) wave functions[2] and the Sternheimer differential equation (DE) procedure[1] for the following isoelectronic series of atoms: B, $C^+$, $N^{2+}$, $O^{3+}$, $F^{4+}$ ($2p^1$, $^2P$ state); C, N, $O^{2+}$, $F^{3+}$, $Ne^{4+}$ ($2p^2$, $^3P$ state); $N^-$, O($2p^4$, $^1D$ state); $N^-$, O, $F^+$, $Ne^{2+}$, $Na^{3+}$, $Mg^{4+}$ ($2p^4$, $^3P$ state); F, $Ne^+$, $Na^{2+}$, $Mg^{3+}$, $Al^{4+}$ ($2p^5$, $^2P$ state); Al, $Si^+$, $P^{2+}$, $S^{3+}$, $Cl^{4+}$ ($3p^1$, $^2P$ state); S($3p^4$, $^1D$ state); S, $Cl^+$, $A^{2+}$, $Ca^{4+}$ ($3p^4$, $^3P$ state); and Cl, $A^+$, $Ca^{3+}$, $Sc^{4+}$ ($3p^5$, $^2P$ state). The present results should add to the $R$ values reported earlier[3] for $Pr^{3+}(4f^2)$, $Tm^{3+}(4f^{12})$, and other rare-earth ions[4]; Cu($3d^9 4s^2$), Cu($3d^{10}4p^1$), Pr($5d$), Tm($5d$), Li($2p^1$), Li($3p^1$), Be($2s2p$)[5]; B($2p$) and Al($2p$)[6]; F($2p^5$), O($2p^4$), Sc($3d$), $Fe^{2+}(3d^6)$, Ga($4p$), and Br($4p^5$)[7]; several alkali metals[8] in the excited $np$ and $nd$ configuration; and a few systems[9] of interest in Mössbauer spectroscopy. In the cases of the free ions the results reported in this paper are new and should be useful in interpreting the relevant experimental data on the quadrupole interaction when they become available. The present calculations should be regarded as the zeroth-order approximation, in electron-electron interaction, to R. More accurate calculations of $R$ including the higher-order effects are available for a few light atoms[10-14] and $Fe^{2+}$ ion.[15]

In Sec. II we present a brief account of the method of calculations adopted by us. Section III contains the results obtained in this work along with the conclusions. Finally, in Sec. IV a summary of the present work is given.

## II. CALCULATIONS

The procedure of calculating $R$ factors in all details is given in Refs. 3 and 5 by Sternheimer. The main step consists in obtaining the nuclear quadrupole moment perturbed radial wave functions $v_1'(nl \to l')$ according to the following inhomogeneous differential equation:

$$\left(-\frac{d^2}{dr^2}+\frac{l'(l'+1)}{r^2}+V_o-E_0\right)v_1'(nl\to l') = u_o'(nl)\left[r^{-3}-\langle r^{-3}\rangle_{nl}\delta_{ll'}\right], \tag{2}$$

where $u_o'(nl)$ defines $r$ times the unperturbed radial wave functions corresponding to the orbital described by the quantum numbers $nl$. The various radial ($l'=l$) and angular ($l'=l\pm 2$) perturbations have been obtained by an iterative numerical integration code described elsewhere.[9] The total $R$ is obtained by adding the direct and exchange contributions between the perturbed charge density and the valence electrons summed over all the $nl \to l'$ perturbations:

$$R=\sum_{nl}\left[R_D(nl\to l')+R_E(nl\to l')\right], \tag{3}$$

where the direct term is given by

$$R_D(nl\to l') = \frac{c(nl\to l')}{\langle r^{-3}\rangle_{n_e l_e}}\int_0^\infty\left(\frac{1}{r^{L+1}}\int_0^r f_1 f_2 r'^{L}\,dr' + r^L\int_r^\infty f_1 f_2 r'^{-L-1}\,dr'\right) f_3 f_4\,dr, \tag{4}$$

with $f_1=u_o'(nl)$, $f_2=v_1'(nl\to l')$, $f_3=f_4$ being the valence wave function $w(n_e l_e)$, and $L=2$. $c(nl\to l')$

gives the result over the angular integrals. For $R_E\ (nl \rightarrow l')$, we have in Eq. (4) $f_1 = v_1'\ (nl \rightarrow l')$, $f_2 = w\ (n_e l_e)$, $f_3 = u_0'\ (nl)$, $f_4 = w(n_e l_e)$, and $C(nl \rightarrow l', L)$, with several allowed values of $L$ which are the angular factors defined by the total exchange interaction. The constants $c$ and $C$ have been tabulated in Ref. 5. We note here that in the case of $p^4$ isoelectric series, $c$'s are multiplied by $\frac{1}{2}$ due to the half-filled shell interacting with a single valence electron with opposite spin.

## III. RESULTS AND DISCUSSION

In Table I we have presented the shellwise contribution to $R$ for the $\mathrm{B}(2p^1)\,^2P$, and $\mathrm{C}(2p^2)\,^3P$ isoelectronic series. The present result of $R = +0.049$ for $B$ is in excellent agreement with the value $+0.048$ obtained by Sternheimer[6] using a modified potential for the valence electron which reproduces the experimental binding energy. A slightly larger value obtained in the present case is due to the HF estimate of $\langle r^{-3}\rangle_{2p} = 0.7758$ a.u., which is somewhat smaller than 0.7798 as calculated by Sternheimer.[6] More accurate calculations[11,12] of $R$ also yield a value of 0.048 for $B$. For the positive ions one expects the higher-order effects to be less important, which means that the $R$ values for the positive ions isoelectronic with $B$ and $C$ as obtained in Table I should be quite reliable. For $\mathrm{C}(2p^2)\,^3P$ the present value of $R = +0.037$ compares reasonably well with the value of $+0.033$ as obtained by Schaefer *et al.*[11] The net values of $R$ for the neutral atom and the isoelectronic positive ions considered in Table I are found to be shielding ($R > 0$). As mentioned before, the total contribution from each shell is a sum of the direct and exchange terms corresponding to a given excitation $nl \rightarrow l'$. In Table I the exchange terms corresponding to $ns \rightarrow d$ excitations are found, in general, to be of the same order as the direct terms with opposite sign. For $2s \rightarrow d$ excitations $R_E \sim R_D$ which is due to the strong overlap between the $2p$ electron wave functions with $u_0'$ and $u_1'$, respectively. Within the isoelectronic series both $R_D$ and $R_E$ (and hence $R$) decrease in magnitude as $Z$ increases. The results in Table I can be used to estimate the change in $R$ with ionicity. For example, the $R$ factor decreases from $+0.0372$ to $+0.0359$ in going from C to $\mathrm{C}^+$. Small decreases of such order can also be noted for the pairs $\mathrm{N}^+$-$\mathrm{N}^{2+}$, $\mathrm{O}^{2\pm}$-$\mathrm{O}^{3+}$, and $\mathrm{F}^{3+}$-$\mathrm{F}^{4+}$ as 0.029 – 0.0290, 0.0238 – 0.0234, and 0.0205 – 0.0200, respectively.

TABLE I. Quadrupole valence shielding factors $R$ for the $\mathrm{B}(^2P)$ and $\mathrm{C}(^3P)$ isoelectronic series. $R_D$, $R_E$, and $R_T$, respectively, denote the direct, exchange, and total contribution due to a given perturbation $nl \rightarrow l'$. All values have been shown as amplified by a factor of $10^2$.

| Atom | $R_D$ | $R_E$ | $R_T$ | $R_D$ | $R_E$ | $R_T$ | $R$ |
|---|---|---|---|---|---|---|---|
| $\mathrm{B}(2p^1)$ :$^2P$ | 9.44 | −4.66 | 4.79 | 3.88 | −3.78 | 0.10 | 4.89 |
| $\mathrm{C}^+$ $^2P$ | 7.35 | −4.01 | 3.34 | 2.43 | −2.19 | 0.24 | 3.59 |
| $\mathrm{N}^{2+}$ $^2P$ | 6.02 | −3.48 | 2.55 | 1.56 | −1.21 | 0.36 | 2.90 |
| $\mathrm{O}^{3+}$ $^2P$ | 5.10 | −3.05 | 2.05 | 1.38 | −1.09 | 0.29 | 2.34 |
| $\mathrm{F}^{4+}$ $^2P$ | 4.43 | −2.72 | 1.71 | 1.12 | −0.84 | 0.28 | 2.00 |
| $\mathrm{C}(2p^2)$ :$^3P$ | 7.53 | −3.93 | 3.60 | 2.79 | −2.66 | 0.13 | 3.72 |
| $\mathrm{N}^+$ $^3P$ | 6.15 | −3.43 | 2.72 | 1.92 | −1.70 | 0.22 | 2.94 |
| $\mathrm{O}^{2+}$ $^3P$ | 5.20 | −3.03 | 2.17 | 1.60 | −1.39 | 0.21 | 2.38 |
| $\mathrm{F}^{3+}$ $^3P$ | 4.50 | −2.70 | 1.80 | 1.22 | −0.97 | 0.25 | 2.05 |
| $\mathrm{Ne}^{4+}$ $^3P$ | 3.92 | −2.43 | 1.49 | 0.98 | −0.73 | 0.25 | 1.74 |

The shellwise contributions to $R$ for O and F series are listed in Table II. Sternheimer[7] has

TABLE II. Quadrupole valence shielding factors $R$ for the $\mathrm{O}(^1D)$, $\mathrm{O}(^3P)$, and $\mathrm{F}(^2P)$ isoelectronic series. The direct, exchange, and total contributions to $R$ due to a given perturbation $nl \rightarrow l'$ are denoted by $R_D$, $R_E$, and $R_T$, respectively. For convenience all entries have been multiplied by $10^2$.

| | $1s \rightarrow d$ | | | $2s \rightarrow d$ | | | $2p \rightarrow f$ | | | $2p \rightarrow p$ | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Atom Perturbation | $R_D$ | $R_E$ | $R_T$ | $R_D$ | $R_E$ | $R_T$ | $R_D$ | $R_E$ | $R_T$ | $R_D$ | $R_E$ | $R_T$ | $R$ |
| $\mathrm{N}^-$ $(2p^4)\,^1D$ | 6.33 | −3.01 | 2.99 | 2.37 | −2.25 | 0.12 | 1.49 | | 1.49 | 9.49 | | 9.49 | 14.09 |
| O $(2p^4)\,^1D$ | 5.36 | −2.96 | 2.40 | 1.77 | −1.61 | 0.16 | 1.35 | | 1.35 | 4.12 | | 4.12 | 8.01 |
| $\mathrm{N}^-$ $(2p^4)\,^3P$ | 6.34 | −3.34 | 3.00 | 2.36 | 2.26 | 0.10 | 1.51 | | 1.51 | 8.63 | | 8.63 | 13.25 |
| O $(2p^4)\,^3P$ | 5.37 | −2.97 | 2.40 | 1.76 | −1.60 | 0.16 | 1.35 | | 1.35 | 3.94 | | | 7.85 |
| $\mathrm{F}^+$ $(2p^4)\,^3P$ | 4.64 | −2.66 | 1.98 | 1.37 | −1.18 | 0.19 | 2.60 | | 2.60 | 1.20 | | | 5.96 |
| $\mathrm{Ne}^{2+}$ $(2p^4)\,^3P$ | 4.08 | −2.41 | 1.68 | 1.18 | −1.00 | 0.18 | 1.94 | | 1.94 | 1.06 | | | 4.87 |
| $\mathrm{Na}^{3+}$ $(2p^4)\,^3P$ | 3.65 | −2.19 | 1.45 | 0.97 | −0.77 | 0.20 | 1.55 | | 1.55 | 0.96 | | | 4.16 |
| $\mathrm{Mg}^{4+}$ $(2p^4)\,^3P$ | 3.29 | −2.02 | 1.28 | 0.84 | −0.64 | 0.20 | 1.29 | | 1.29 | 0.87 | | | 3.63 |
| F $(2p^5)\,^2P$ | 4.69 | −2.64 | 2.05 | 1.48 | −1.33 | 0.15 | 2.33 | −1.16 | 1.16 | 7.35 | −0.61 | 6.74 | 1.01 |
| $\mathrm{Ne}^+$ $(2p^5)\,^2P$ | 4.13 | −2.39 | 1.74 | 1.13 | −0.93 | 0.20 | 2.10 | −1.05 | 1.05 | 4.99 | −0.42 | 4.57 | 0.76 |
| $\mathrm{Na}^{2+}$ $(2p^5)\,^2P$ | 3.68 | −2.18 | 1.50 | 1.03 | −0.86 | 0.17 | 1.90 | −0.95 | 0.95 | 3.78 | −0.32 | 3.46 | 0.61 |
| $\mathrm{Mg}^{3+}$ $(2p^5)\,^2P$ | 3.33 | −2.01 | 1.32 | 0.89 | −0.71 | 1.18 | 1.72 | −0.86 | 0.86 | 3.04 | −0.25 | 2.79 | 0.52 |
| $\mathrm{Al}^{4+}$ $(2p^5)\,^2P$ | 3.03 | −1.86 | 1.17 | 0.79 | −0.61 | 0.17 | 1.58 | −0.79 | 0.79 | 2.54 | −0.21 | 2.33 | 0.45 |

TABLE III. Quadrupole valence shielding factors $R$ for Al $^2P$, S $^3P$, Cl $^2P$ isoelectronic series and S($^1D$) atom. Corresponding to each perturbation $nl \rightarrow l'$ the net contribution $R_T$ given by $R_D + R_E$ is shown. All values are multiplied by a factor of $10^2$ for convenience.

| Atom | $1s \rightarrow d$ | $2s \rightarrow d$ | $3s \rightarrow d$ | $2p \rightarrow f$ | $3p \rightarrow f$ | $2p \rightarrow p$ | $3p \rightarrow p$ | $R$ |
|---|---|---|---|---|---|---|---|---|
| Al($3p^1$) $^2P$ | 1.21 | 1.24 | −0.05 | 1.81 | | −11.71 | | −7.50 |
| Si$^+$ | 1.04 | 1.00 | −0.06 | 1.49 | | −7.48 | | −4.02 |
| P$^{2+}$ | 0.91 | 0.86 | −0.04 | 1.27 | | −5.63 | | −2.63 |
| S$^{3+}$ | 0.82 | 0.76 | −0.02 | 1.13 | | −4.41 | | −1.73 |
| Cl$^{4+}$ | 0.74 | 0.65 | −0.00 | 1.02 | | −3.60 | | −1.20 |
| S ($3p^4$) $^1D$ | 0.85 | 0.83 | −0.04 | 1.24 | 0.40 | −5.51 | 3.89 | 1.66 |
| S ($3p^4$) $^3P$ | 0.85 | 0.84 | −0.04 | 1.24 | 0.40 | −5.56 | 3.73 | 1.47 |
| Cl$^+$ | 0.77 | 0.74 | −0.03 | 1.11 | 0.35 | −4.45 | 2.41 | 0.94 |
| A$^{2+}$ | 0.70 | 0.66 | −0.02 | 1.00 | 0.32 | −3.67 | 2.08 | 0.87 |
| Ca$^{4+}$ | 0.59 | 0.55 | 0.00 | 0.85 | 0.25 | −2.69 | 1.01 | 0.55 |
| Cl($3p^5$) $^2P$ | 0.77 | 0.76 | −0.03 | 1.13 | 0.35 | −4.70 | 5.69 | 3.97 |
| A$^+$ | 0.70 | 0.68 | −0.02 | 1.02 | 0.32 | −3.88 | 4.34 | 3.17 |
| Ca$^{3+}$ | 0.60 | 0.56 | 0.03 | 0.86 | 0.26 | −2.83 | 2.61 | 2.13 |
| Sc$^{4+}$ | 0.55 | 0.52 | 0.09 | 0.80 | 0.24 | −2.48 | 2.03 | 1.75 |

earlier calculated $R$ for O and F atoms as 0.0781 and 0.1075, respectively. Our results for these two systems are 0.0785 and 0.101, respectively, which are almost in exact agreement with the calculations of Sternheimer. The general trends noted before with respect to the variation of $R_D$, $R_E$, and $R$, respectively, in the B and C isoelectronic series also hold good for the O and F series. The $R$ factors for the negative ions are calculated to be almost twice the magnitude of the isoelectronic neutral atom. This is due to more external valence electron wave functions of the negative ions. We have also calculated $R$ for N$^-$ and O in $^1D$ and $^3P$ atomic states, respectively, in order to see if there exists a differential shielding effect at the zeroth order in electron-electron interaction. It is found that the $R$ factor corresponding to the $^1D$ state is always slightly larger in magnitude. For example, for N$^-$ and O in the $^1D$ state, $R = +0.1409$ and $+0.0801$, as compared to the $^3P$-state results of $+0.1325$ and $+0.0785$, respectively.

In Table III we have presented the total $(R_D + R_E)$ shellwise contribution to $R$ for the Al($3p^1$, $^2P$), S($3p^4$, $^3P$), and Cl($3p^5$, $^2P$) isoelectronic series. The present value of $R$ for Al is calculated to be −0.0750 which differs somewhat in magnitude from the previous result[6] of −0.063 wherein a modified potential for the $3p$ electron is used which reproduces the experimental $3p$ binding energy. The $\langle r^{-3}\rangle_{3p}$ value obtained in this way is 1.2960 $a_H^{-3}$, which is 1.19 times the presently calculated value of 1.093 $a_H^{-3}$ using the HF wave functions of Clementi and Roetti.[2] Since $\langle r^{-3}\rangle_{3p}$ appears in the denominator of $R$, the present result should be multiplied by[1] 1.19 and then compared with the result in Ref. 6. With such a scaling our result be-

TABLE IV. Values of $\langle r^{-3}\rangle_{\text{val}}$ (in $a_H^{-3}$ units), $R$, and $(1-R)^{-1}$ corresponding to the $2p$ and $3p$ atoms and ions.

| Atom | $\langle r^{-3}\rangle_{\text{val}}$ | $R$ | $(1-R)^{-1}$ |
|---|---|---|---|
| B $^2P$ | 0.776 | 0.049 | 1.052 |
| C$^+$ | 2.221 | 0.036 | 1.037 |
| N$^{2+}$ | 4.677 | 0.029 | 1.030 |
| O$^{3+}$ | 8.396 | 0.023 | 1.024 |
| F$^{4+}$ | 13.629 | 0.020 | 1.020 |
| C $^3P$ | 1.692 | 0.037 | 1.038 |
| N$^+$ | 3.834 | 0.029 | 1.030 |
| O$^{2+}$ | 7.168 | 0.024 | 1.025 |
| F$^{3+}$ | 11.943 | 0.021 | 1.022 |
| Ne$^{4+}$ | 18.998 | 0.017 | 1.017 |
| N- $^1$D | 2.333 | 0.141 | 1.164 |
| O | 4.920 | 0.080 | 1.087 |
| N- $^3P$ | 2.368 | 0.133 | 1.153 |
| O | 4.970 | 0.079 | 1.086 |
| F$^+$ | 8.861 | 0.060 | 1.064 |
| Ne$^{2+}$ | 14.293 | 0.049 | 1.052 |
| Na$^{3+}$ | 21.769 | 0.042 | 1.044 |
| Mg$^{4+}$ | 30.798 | 0.036 | 1.037 |
| F $^2P$ | 7.541 | 0.010 | 1.010 |
| Ne$^+$ | 12.485 | 0.008 | 1.008 |
| Na$^{2+}$ | 19.156 | 0.006 | 1.006 |
| Mg$^{3+}$ | 27.803 | 0.005 | 1.005 |
| Al$^{4+}$ | 38.661 | 0.005 | 1.005 |
| Al $^2P$ | 1.093 | −0.075 | 0.930 |
| Si$^+$ | 2.639 | −0.040 | 0.962 |
| P$^{2+}$ | 4.818 | −0.026 | 0.975 |
| S$^{3+}$ | 7.689 | −0.017 | 0.983 |
| Cl$^{4+}$ | 11.317 | −0.012 | 0.988 |
| S $^1D$ | 4.836 | 0.017 | 1.017 |
| S $^3P$ | 4.841 | 0.015 | 1.015 |
| Cl$^+$ | 7.791 | 0.009 | 1.009 |
| A$^{2+}$ | 11.530 | 0.009 | 1.009 |
| Ca$^{4+}$ | 21.638 | 0.006 | 1.006 |
| Cl $^2P$ | 6.767 | 0.040 | 1.042 |
| A$^+$ | 10.275 | 0.032 | 1.033 |
| Ca$^{3+}$ | 19.884 | 0.021 | 1.021 |
| Sc$^{4+}$ | 26.090 | 0.018 | 1.018 |

comes $-0.063$, which is in exact agreement with previous calculation.[6] In the case of S no estimates of $R$ are available in the literature. For the $^1D$ and $^3P$ states of $S(3p^4)$ the present values are $+0.0166$ and $+0.0147$, respectively, which indicates a differential shielding effect similar to that found in the cases of $N^-$ and O, respectively. For $Cl(3p^5)$ the presently calculated $R=0.040$ is also in good agreement with Sternheimer's[7] result of 0.043. The corresponding values of $\langle r^{-3}\rangle$ are also very nearly the same, i.e., $6.77a_H^{-3}$ and $6.76a_H^{-3}$, respectively.

The $3p$ atoms and ions are characterized by the net antishielding arising from $2p \to p$ excitation. In the case of Al series this results in $R$, which is antishielding. Another special feature of these systems is the near cancellation of $R_D$ and $R_E$ corresponding to the $3s \to d$ excitations in general. For S and Cl series $R$ is found to be shielding due to the significantly positive contribution from the $3p$ shell. The variation of $R$ with $Z$ within an isoelectronic series is found to be similar to the $2p$ series of atoms, i.e., $R$ decreases with increase in $Z$.

## IV. SUMMARY

In Table IV we have compiled the values of $R$, $(1-R)^{-1}$, and $\langle r^{-3}\rangle_{\rm val}$ obtained in this work. The main conclusions derived from our work can be summarized as follows: (a) the total $R$ for $2p$ and $3p$ atoms and ions are shielding except for the $Al(3p^1)$-like systems where an antishielding effect is obtained; (b) the $R$ values for the mononegative ions are found to be almost twice as large as the isoelectronic neutral atom; (c) for the same atom, $R$ corresponding to $^1D$ state is found to be slightly larger than that in the $^3P$ state; and (d) within an isoelectronic series, $R$ decreases with increase in $Z$, the atomic number.

*Note added in proof.* In a very recent paper [S. Lauer, V. R. Marathe, and A. Trautwein, Phys. Rev. A 19, 1852 (1979)] on the calculations of $R$ it has been noted that the use of angular coefficients[5] adopted in the present work is justified when the associated $\langle r^{-3}\rangle_{\rm val}$ have been estimated using the magnetic hyperfine structure interval data. The present results should be used with this requirement in view.

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