# SCALAR AND TENSOR POLARIZABILITIES OF LOW LYING S, P, D, F AND G STATES IN RUBIDIUM

W. A. VAN WIJNGAARDEN

Department of Physics, York University, 4700 Keele Street, Toronto, Ontario, Canada M3J 1P3

**Abstract**—The scalar and tensor polarizabilities of over 50 of the lowest $S$, $P$, $D$, $F$ and $G$ states of rubidium are evaluated using a Coulomb approximation. The computed results are in good agreement with measured values found in the literature which are briefly reviewed. The scalar polarizability $\alpha_o$ of the $(5-12)S_{1/2}$ states is found to be given to within 2% by the formula $\alpha_o/n^{*7} = 0.267 + 8.69/n^*$ where $n^*$ is the effective principal quantum number. © 1997 Elsevier Science Ltd. All rights reserved

## 1. INTRODUCTION

Polarizabilities of atomic states govern the response of an atom to an electric field. Accurate measurements of polarizabilities yield information about atomic structure that is required to describe charge-exchange cross sections, van der Waals constants and dielectric constants.[1-3] Recently, interest in polarizabilities has increased due to highly accurate measurements of transition Stark shifts.[4] The latter are important for testing atomic theory as well as for applications such as the measurement of electrode spacings[5] and the determination of electric fields in plasmas.[6]

Much experimental and theoretical work has been done on alkali atoms. These atoms have only a single valence electron permitting the interaction of the outer electron with the nucleus and the inner core electrons to be well modelled by a Coulomb potential. This so-called Coulomb approximation[7] has been used to compute polarizabilities of low lying states in sodium, potassium, and cesium.[8,9] The computed results have been found to agree with the experimental data to a few percent. This method has the advantage of being much simpler than more elaborate many body calculations[10] and therefore requires substantially less computational effort. This paper reports the scalar and tensor polarizabilities of over 50 of the lowest lying states in rubidium. The results agree well with the experimental measurements which are reviewed. Rubidium is important in a number of applications including frequency and wavelength standards[11,12] and was recently used to observe Bose Einstein condensation.[13]

The Hamiltonian describing the effect of an electric field $E$ on an atom is given by[14]

$$H = -\left\{\alpha_o + \alpha_2 \frac{3J_z^2 - \mathbf{J}^2}{J(2J-1)}\right\} \frac{E^2}{2} \tag{1}$$

where $\mathbf{J}$ is the electronic angular momentum and the quantization axis $z$ is parallel to the field direction. The second term vanishes when $J < 1$. $\alpha_o$ and $\alpha_2$ are the scalar and tensor polarizabilities respectively and are defined by

$$\alpha_o = \frac{r_o}{4\pi^2} \sum_{J'} \lambda_{JJ'}^2 f_{JJ'} \tag{2}$$

$$\alpha_2 = \frac{r_o}{8\pi^2} \frac{1}{(2J+3)(J+1)} \sum_{J'} \lambda_{JJ'}^2 f_{JJ'}[8J(J+1) - 3X(X+1)] \tag{3}$$

where $X = J'(J' + 1) - 2 - J(J + 1)$. $r_o$ is the classical electron radius, $\lambda_{JJ'}$ is the wavelength for a transition between states $J$ and $J'$ and $f_{JJ'}$ is the transition oscillator strength.

Table 1 lists polarizabilities computed using the Coulomb approximation of Bates and Damgaard which is discussed in detail in Refs. 7 and 8. These results were found using the excited state energies determined by Moore.[15] The polarizabilities are predicted to scale as $n^{*7}$ where $n^*$ is the effective principle quantum number[16] for states having a small fine structure and a minimal

Table 1. Computed polarizabilities. Note that 1 kHz/$(kV/cm)^2 = 4.0189\, a_o^3/h$ and $a_o^3 = 1.4818 \times 10^{-25}\,cm^3$ where $a_o$ is the Bohr radius and $h$ is Planck's constant.

| State | $n^*$ | $\alpha_o(a_o^3)$ | $\alpha_2(a_o^3)$ |
|---|---|---|---|
| $5S_{1/2}$ | 1.805 | $3.14E2$ | |
| $6S_{1/2}$ | 2.845 | $5.11E3$ | |
| $7S_{1/2}$ | 3.856 | $3.24E4$ | |
| $8S_{1/2}$ | 4.861 | $1.32E5$ | |
| $9S_{1/2}$ | 5.863 | $4.16E5$ | |
| $10S_{1/2}$ | 6.865 | $1.09E6$ | |
| $11S_{1/2}$ | 7.865 | $2.51E6$ | |
| $12S_{1/2}$ | 8.866 | $5.26E6$ | |
| $5P_{1/2}$ | 2.280 | $8.05E2$ | |
| $6P_{1/2}$ | 3.317 | $1.26E4$ | |
| $7P_{1/2}$ | 4.329 | $8.36E4$ | |
| $8P_{1/2}$ | 5.335 | $3.60E5$ | |
| $9P_{1/2}$ | 6.338 | $1.19E6$ | |
| $10P_{1/2}$ | 7.339 | $3.26E6$ | |
| $11P_{1/2}$ | 8.340 | $7.82E6$ | |
| $12P_{1/2}$ | 9.341 | $1.37E7$ | |
| $13P_{1/2}$ | 10.342 | $3.46E7$ | |
| $5P_{3/2}$ | 2.293 | $8.68E2$ | $-1.43E2$ |
| $6P_{3/2}$ | 3.330 | $1.36E4$ | $-2.04E3$ |
| $7P_{3/2}$ | 4.342 | $9.06E4$ | $-1.25E4$ |
| $8P_{3/2}$ | 5.348 | $3.91E5$ | $-5.08E4$ |
| $9P_{3/2}$ | 6.351 | $1.29E6$ | $-1.60E5$ |
| $10P_{3/2}$ | 7.353 | $3.55E6$ | $-4.24E5$ |
| $11P_{3/2}$ | 8.354 | $8.54E6$ | $-9.74E5$ |
| $12P_{3/2}$ | 9.354 | $1.51E7$ | $1.42E6$ |
| $13P_{3/2}$ | 10.355 | $3.70E7$ | $-3.66E6$ |
| $4D_{3/2}$ | 2.767 | $5.71E2$ | $-4.90E1$ |
| $5D_{3/2}$ | 3.709 | $1.87E4$ | $-1.30E3$ |
| $6D_{3/2}$ | 4.683 | $9.60E4$ | $-5.59E2$ |
| $7D_{3/2}$ | 5.672 | $3.35E5$ | $1.86E4$ |
| $8D_{3/2}$ | 6.666 | $9.36E5$ | $1.05E5$ |
| $9D_{3/2}$ | 7.662 | $2.26E6$ | $3.73E5$ |
| $10D_{3/2}$ | 8.660 | $-4.85E6$ | $2.99E6$ |
| $11D_{3/2}$ | 9.658 | $9.35E6$ | $6.33E6$ |
| $4D_{5/2}$ | 2.767 | $5.35E2$ | $-1.83E1$ |
| $5D_{5/2}$ | 3.707 | $1.83E4$ | $-1.20E3$ |
| $6D_{5/2}$ | 4.684 | $9.36E4$ | $3.45E3$ |
| $7D_{5/2}$ | 5.673 | $3.25E5$ | $4.48E4$ |
| $8D_{5/2}$ | 6.667 | $9.04E5$ | $2.11E5$ |
| $9D_{5/2}$ | 7.664 | $2.17E6$ | $7.01E5$ |
| $10D_{5/2}$ | 8.661 | $-5.14E6$ | $4.70E6$ |
| $11D_{5/2}$ | 9.659 | $-9.99E6$ | $9.98E6$ |
| $4F_{5/2}$ | 3.988 | $-4.53E3$ | $9.30E3$ |
| $5F_{5/2}$ | 4.986 | $2.08E6$ | $-7.00E5$ |
| $6F_{5/2}$ | 5.985 | $1.46E7$ | $-5.04E6$ |
| $7F_{5/2}$ | 6.984 | $-9.95E5$ | $8.50E5$ |
| $8F_{5/2}$ | 7.984 | $-2.56E6$ | $2.19E6$ |
| $4F_{7/2}$ | 3.988 | $-4.58E3$ | $1.09E4$ |
| $5F_{7/2}$ | 4.986 | $2.08E6$ | $-8.16E5$ |
| $6F_{7/2}$ | 5.985 | $1.45E7$ | $-5.87E6$ |
| $7F_{7/2}$ | 6.984 | $-1.00E6$ | $1.00E6$ |
| $8F_{7/2}$ | 7.984 | $-2.58E6$ | $2.58E6$ |
| $5G_{7/2}$ | 4.998 | $1.63E6$ | $1.51E6$ |
| $6G_{7/2}$ | 5.994 | $-5.12E5$ | $5.46E6$ |
| $5G_{9/2}$ | 4.998 | $-1.63E6$ | $1.65E6$ |
| $6G_{9/2}$ | 5.994 | $-5.00E5$ | $5.94E6$ |
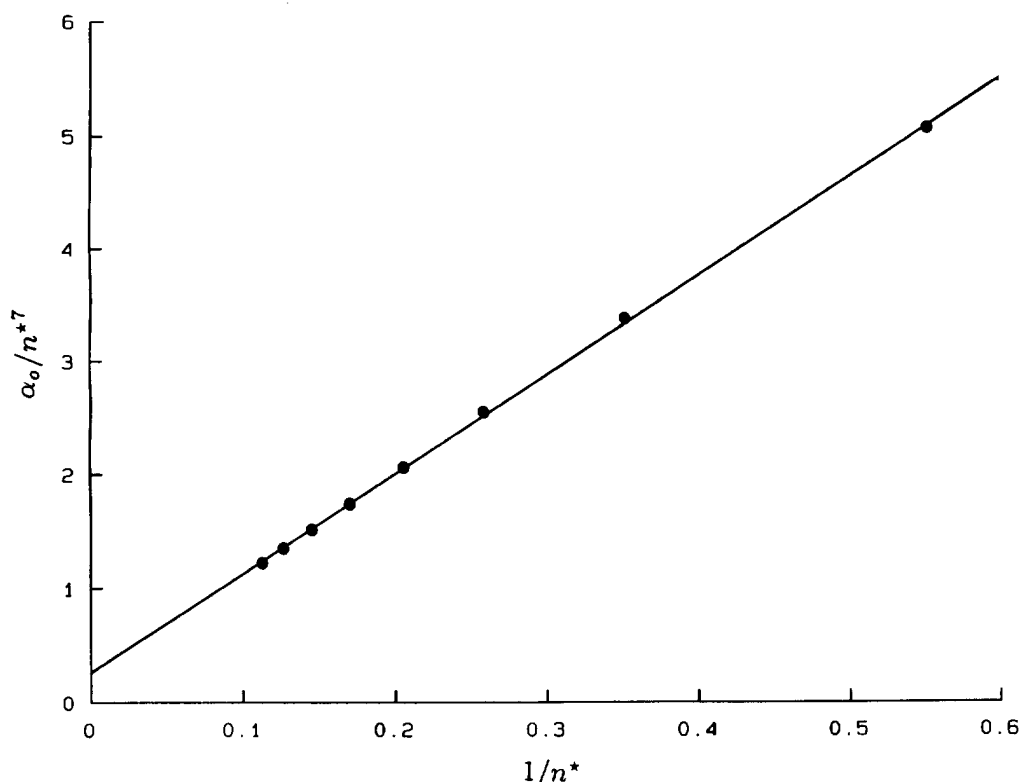
Fig. 1. Dependence of scalar polarizability for the $(5-12)S_{1/2}$ states on effective principal quantum number $n^*$. The dots are found using the data listed in Table 1. The curve best fitting the data is given by $\alpha/n^{*7} = 0.267 + 8.69/n^*$ as is discussed in the text.

penetration of the inner electron core. This is found to be the case for the $(5-12)S_{1/2}$ states as is shown in Fig. 1 where $\alpha_o/n^{*7}$ is plotted versus $1/n^*$. A least squares fit of the function

$$\alpha/n^{*7} = A + B/n^* \tag{4}$$

to the data yielded $A = 0.267$ and $B = 8.69$. The values obtained for the polarizabilities using the fitted constants agreed with the theoretical results given in Table 1 to better than 2%.

The polarizabilities of some highly excited states having principal quantum number between 15 and 80 have been investigated using two photon excitation by O'Sullivan and Stoicheff.[17] A narrow linewidth dye laser excited rubidium atoms contained in two cells. An electric field was applied to one cell. The fluorescence produced by the radiative decay of the excited state was monitored as the laser frequency was scanned across the resonance. The change in laser frequency was monitored by passing part of the laser beam through a Fabry Perot etalon. A fit of their data to Eq. (4) yielded values of $A = 0.222$ and $B = 8.85$. The agreement with the result of this paper is reasonable considering that $\alpha_o(80S_{1/2})$ is more than ten orders of magnitude larger than $\alpha_o(5S_{1/2})$. Indeed, the value of $\alpha_o(80S_{1/2})$ obtained using the scaling formula fitted to the data for the $(5-12)S_{1/2}$ states is $6.02 \times 10^{12}a_o^3$ where $a_o$ is the Bohr radius. This compares to $(5.39 \pm 0.53) \times 10^{12}a_o^3$ as measured by O'Sullivan and Stoicheff.

Table 2 contains a list of measured polarizabilities. Hall and Zorn[18] determined the ground state polarizability by measuring the deflection of a neutral atomic beam by an inhomogeneous electric field. A more accurate result was obtained by Molof et al[19] using both inhomogeneous magnetic and electric fields. The atomic beam was not deflected when the magnetic and electric forces cancel i.e. $\alpha E\, dE/dz = \mu\, dH/dz$. The polarizability was then found using the known field gradients and the ground state magnetic moment $\mu$. The foregoing methods are best suited for studying the ground state since atomic beams having nearly all atoms in their lowest state are readily generated.

Several groups have studied excited states using level crossing spectroscopy.[14,20-22] This method uses light produced by either a laser or a rf discharge lamp to excite an atomic beam or atoms

stored in a vapor cell. Atomic beams are preferable since cell walls may strongly perturb the electric field. The fluorescence is then detected by a photomultiplier as a function of the electric and/or magnetic field. The fields shift the energies of the various hyperfine levels changing the fluorescence polarization. This effect is largest whenever the energy of two excited state hyperfine levels are degenerate or are said to cross. This method determines only the tensor polarizability since the scalar polarizability shifts all hyperfine levels encompassing the fine structure manifold of an excited state equally. The accuracy of the resulting data is generally limited by uncertainties in the determination of the electric field.

The level crossing method was first employed by Khadjavi et al[14] who excited an atomic beam of rubidium atoms to the $5P_{3/2}$ state using light produced by a discharge lamp. The electric field was generated by two stainless steel plates separated by two quartz spacers. Fluorescence, generated by the radiative decay of the excited state back to the ground state was detected by a photomultiplier while the electric field was scanned from 0 to 15 kV/cm. The tensor polarizability was found by measuring the electric fields where the level crossings occurred.

A similar experiment has been done by Svanberg[21] who studied the $5P_{1/2}$ and $7P_{1/2}$ states. Level crossing signals were first recorded by measuring the fluorescence polarization as a function of an applied magnetic field in the absence of an electric field. The experiment was then repeated at a finite electric field to measure the shift of the level crossing positions. The tensor polarizability was obtained using the hyperfine splitting and the Lande $g$ value of the excited $P_{1/2}$ state. The advantage of this experiment is that the electric fields were less than 1 kV/cm as compared to as high as 15 kV/cm in the work done by Khadjavi et al. Hogervorst and Svanberg[22] extended their work using a dye laser to excite the $5P_{1/2}$ or $5P_{3/2}$ states to study the $(6-9)D_{3/2,5/2}$ states.

The scalar polarizabilities of some excited states have been found by Fredriksson and Svanberg.[23] The atoms were first excited to the $5P_{1/2}$ state by a lamp as in their earlier work. A dye laser was then tuned close to the frequency of a transition from the $5P_{1/2}$ state to one of the $(9-10)S_{1/2}$ or $(6-8)D_{3/2}$ states. Fluorescence produced by the radiative decay of the excited state was detected by a photomultiplier and recorded as the electric field was increased from zero. The electric fields needed to bring into resonance the two hyperfine levels of the $5P_{1/2}$ state were then measured. The scalar polarizabilities of the $(9-10)S_{1/2}$ or $(6-8)D_{3/2}$ states were obtained using the known hyperfine splitting of the $5P_{1/2}$ state. For the $(6-8)D_{3/2}$ states, one also needed the tensor polarizability which had been determined previously using level crossing spectroscopy.

A comparison of the computed results listed in Table 1 and the experimental measurements in Table 2 show good agreement except for some of the lowest excited states such as the $6D_{3/2,5/2}$ states. This is not surprising since the valence electron penetration of the inner electron core for these states is not adequately considered by the Coulomb approximation. The computed results for the higher $(7-9)D_{3/2,5/2}$ states are in closer agreement with the experimental data as is expected since the valence electron for these states is further from the nucleus than is the case for the $6D_{3/2,5/2}$ states.

Table 2. Measured scalar and tensor polarizabilities. Note that $1 \text{ kHz}/(\text{kV/cm})^2 = 4.0189 \ a_o^3/h$ and $a_o^3 = 1.4818 \times 10^{-25} \text{ cm}^3$ where $a_o$ is the Bohr radius and $h$ is Planck's constant.

| State | $\alpha_o(a_o^3)$ | $\alpha_2(a_o^3)$ | Reference |
|-------|-------------------|-------------------|-----------|
| $5S_{1/2}$ | $(3.29 \pm 0.23)E2$ | | 18 |
| | $(3.19 \pm 0.06)E2$ | | 19 |
| $9S_{1/2}$ | $(4.10 \pm 0.36)E5$ | | 23 |
| $10S_{1/2}$ | $(1.13 \pm 0.10)E6$ | | 23 |
| $6P_{1/2}$ | $(1.04 \pm 0.08)E4$ | | 20 |
| $5P_{3/2}$ | | $(-1.60 \pm 0.24)E2$ | 21 |
| $6P_{3/2}$ | | $(-2.09 \pm 0.08)E3$ | 14 |
| $7P_{3/2}$ | | $(-1.29 \pm 0.08)E4$ | 21 |
| $6D_{3/2}$ | $(1.00 \pm 0.04)E5$ | $(-4.22 \pm 0.28)E2$ | 22 |
| $7D_{3/2}$ | $(3.38 \pm 0.24)E5$ | $(1.99 \pm 0.10)E4$ | 22, 23 |
| $8D_{3/2}$ | $(8.48 \pm 0.72)E5$ | $(1.09 \pm 0.06)E5$ | 22, 23 |
| $6D_{5/2}$ | | $(3.78 \pm 0.20)E3$ | 22 |
| $7D_{5/2}$ | | $(4.78 \pm 0.24)E$ | 22 |
| $8D_{5/2}$ | | $(2.29 \pm 0.12)E5$ | 22 |
| $9D_{5/2}$ | | $(7.25 \pm 0.36)E5$ | 22 |

A stringent test of the theoretical results is presented by the experiment by Miller et al[24] who measured the Stark shift of the rubidium $D_1$ line. This was done using two diode lasers. One laser was locked to the $D_1$ line observed using the saturated absorption signal observed in a cell while the second laser excited an atomic beam as it passed through an electric field. The electric field was generated using two optical quartz flats that formed a Fabry Perot etalon. Part of each of the two diode lasers was then focused onto a fast photodiode. The beat frequency was then measured as a function of the electric field to determine the transition Stark shift yielding

$$\alpha_o(5P_{1/2}) - \alpha_o(5S_{1/2}) = 491.54 \pm 0.06 a_o^3 \tag{6}$$

This is in excellent agreement with the value of 491 $a_o^3$ obtained using the results given in Table 1.

In conclusion, scalar and tensor polarizabilities have been computed using a Coulomb approximation for over 50 of the lowest $S$, $P$, $D$, $F$ and $G$ states in rubidium. The data were compared to experimental results obtained for 14 different states. Good agreement was found giving confidence in the reliability of the theoretical estimates for the states for which no experimental work presently exists. The scalar polarizability of the $S_{1/2}$ states is given by a simple scaling relation involving the effective principal quantum number $n^*$.

## REFERENCES

1. K. D. Bonin and M. A. Kadar-Kallen, *Phys. Rev. A* **47**, 944 (1993).
2. T. M. Miller and B. Bederson, *Adv. Atom. Molecul. Phys.* **13**, 1 (1977).
3. T. M. Miller and B. Bederson, *Adv. Atom. Molec. Opt. Phys.* **25**, 37 (1988).
4. W. A. van Wijngaarden, *Adv. Atom. Molec. Opt. Phys.*, in press.
5. C. Neureiter, R. H. Rinkleff, and L. Windholz, *J. Phys. B* **19**, 2227 (1986).
6. J. E. Lawler and D. A. Doughty, *Advances in Atomic, Molecular and Optical Physics*, B. Bederson and H. Walther, eds., **34**, 171 Academic Press, San Diego (1995).
7. D. R. Bates and A. Damgaard, *Phil. Trans. R. Soc.* **242**, 101 (1949).
8. W. A. van Wijngaarden and J. Li, *JQSRT* **52**, 555 (1994).
9. P. F. Gruzdev, G. W. Soloveva, and A. I. Sherstyuk, *Opt. Spectrosc.* **71**, 513 (1991).
10. I. Lindgren and J. Morrison, *Atomic Many Body Theory*, Springer, Berlin (1986).
11. M. Hashimoto and M. Ohtsu, *JOSA B* **6**, 1777 (1989).
12. C. J. Sansonetti and K. H. Weber, *JOSA B* **2**, 1385 (1985).
13. M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell, *Science* **269**, 198 (1995).
14. A. Khadjavi, A. Lurio, and W. Happer, *Phys. Rev.* **167**, 128 (1968).
15. C. E. Moore, *Atomic Energy Levels*, NSRDS-NBS 35 (1971).
16. H. A. Bethe and E. E. Salpeter, *Quantum Mechanics Of One and Two-Electron Atoms*, Plenum, New York (1977).
17. M. S. O'Sullivan and B. P. Stoicheff, *Phys. Rev. A* **31**, 2718 (1984); *ibid*. **33**, 1640 (1985).
18. W. D. Hall and J. C. Zorn, *Phys. Rev. A* **10**, 1141 (1974).
19. R. W. Molof, H. L. Schwartz, T. M. Miller, and B. Bederson, *Phys. Rev. A* **10**, 1131 (1974).
20. E. S. Polzik and M. P. Chaika, *Opt. Spectrosc.* **52**, 6 (1982).
21. S. Svanberg, *Phys. Scr.* **5**, 132 (1972).
22. W. Hogervorst and S. Svanberg, *Phys. Scr.* **12**, 67 (1975).
23. K. Fredriksson and S. Svanberg, *Z. Phys. A* **281**, 189 (1977).
24. K. E. Miller, D. Krause, and L. R. Hunter, *Phys. Rev. A* **49**, 113 (1994).