OSCILLATOR STRENGTH FOR THE 3s3p^2 3S−3s3p 3P TRANSITION IN Al I

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ABSTRACT

The oscillator strength for the transition 1s^22s2p^3s3p^3 P_{3/2,1/2}^-1s^22s2p^3s3p^2 3S_{1/2} of Al I has been calculated. A potential was obtained which allowed a numerical solution of the Schrödinger equation for the ground- and excited-state wave functions. An f-value of 0.34 was computed from both the dipole and the momentum matrix elements, using theoretical energy levels. This is thought to be a more reliable value than that derived from observed energies.

I. INTRODUCTION

Rocket observations of solar ultraviolet spectra show the strong absorption lines of Al I at 1936.44 and 1931.92 A (McAllister 1959). These lines correspond to the doublet 3s^3p^3 P_{3/2,1/2}^-3s3p^2 3S_{1/2}. As can be seen in Figure 1, these lines are clearly the most distinct features in this region of the solar spectrum. Burgess, Field, and Michie (1960) have recently discussed this transition in connection with the possibility of observing interstellar aluminum.

The abbreviated energy-level diagram in Figure 2 shows the transitions under consideration. It should be noted that the excited state of the transition lies above the series limit for the 3s3p configuration. From this we see that the Al I atom can be aut ionized by the radiationless transition of an electron from the 3s3p^2 3S level to the 3S continuum. The broadening of the 1932 and 1936 A lines, as well as the general depression of the adjacent continuum, can be accounted for by the short lifetime of the 3S level toward this aut ionization process.

II. METHOD AND RESULTS

We have calculated the oscillator strength of the 3s^3p−3s3p^3 configuration from both the dipole and the momentum matrix elements. For this it was necessary to know the wave function of each configuration. The upper configuration was considered approximately as a 3p electron moving in the field of Al II 3s3p, and the ground state was considered as a 3s electron moving in the same field. The potential due to a 3s3p configuration was obtained by modifying a potential given by Biermann and Harting for a self-consistent field for Al II (Biermann and Harting 1943). They tabulate the effective charge due to each of the electrons in the 3s configuration of Al II. This allowed us to obtain the effective charge of the 1s^22s^22p^3s configuration. The effective charge of the 3p electron was calculated by

\[ Z_p(\rho) = e \int_{\rho}^{\infty} \frac{Z(\rho)}{\rho^2} d\rho, \]

where

\[ Z(\rho) = \int_{0}^{\rho} R^3 d\rho, \]

R being the radial wave function and \( \rho \) the distance (all quantities in atomic units). The 3p wave function used in equation (2) was calculated by Münch and Zirin (1960), also based on Biermann and Harting (1943). The effective charge of the 3p electron was then combined with that of the 1s^22s^22p^3s configuration to give the necessary 3s3p
potential. The potential is shown in Figure 3. Using this potential, a numerical integration of the radial Schrödinger equation yielded the wave functions for the ground and excited states of the atom. The numerical integrations for this step were carried out on a digital computer by the method of Clippinger and Dimsdale (Kunz 1957). The energy was varied until wave functions were generated which were consistent with the angular momentum of the electron and which fitted a decreasing exponential at the WKB turning point. The energies which gave satisfactory solutions (called "theoretical energy") were the following: ground state—theoretical energy, −8.13 ev, observed energy, −5.98; excited state—theoretical energy, −4.30 ev, observed energy, +0.43. The wave functions are plotted in Figure 3. We note that the energies necessary to solve the Schrödinger equation do not correspond to the observed levels; they are, however, the values which give proper wave functions for a consistent solution. The observed energy of the excited state is positive (Moore 1949), but a bound-wave-function would not be obtained if a positive energy was used. There are several 3s3p² terms with negative energy, and our method does not distinguish between terms.

The oscillator strength is obtained from the dipole moment matrix element by

\[
f = \frac{1}{3} \frac{\nu}{R_y} \max \frac{(l_L, l_U)}{2l_L + 1} \left( \int_0^\infty R_L R_U d\rho \right)^2
\]

and from the momentum matrix element by

\[
f = \frac{4}{3} \frac{\nu}{R_y} \max \frac{(l_L, l_U)}{2l_L + 1} \left[ \int_0^\infty \left( R_L \frac{dR_U}{d\rho} + \frac{l_U}{R_U} \frac{R_L R_U}{\rho} \right) d\rho \right]^2
\]

where \( \nu \) is the wave number of the transition; \( R_y \) is the Rydberg constant expressed in wave numbers; max \( (l_U, l_L) \) is the larger of \( l_U \) and \( l_L \), where the subscripts refer to the

| OSCILLATOR STRENGTHS FOR THE TRANSITION |
|---|---|---|---|
| Method | Using Theoretical Energy | Using Observed Energy | 1 - D |
| Dipole moment | 347 | 582 | 0.99 |
| Dipole momentum | 340 | 203 | . |

lower and upper states, respectively; \( [] \) is \( l_U \) if \( l_U \) is greater than \( l_L \) and is \(-l_L \) if \( l_U \) is less than \( l_L \). These equations were taken from Green and Weber (1950). Oscillator strengths obtained by these equations are listed in the accompanying table; values are given which were calculated by using the wave number corresponding to both the theoretical and the observed energies. The quantity \( 1 - D \), as discussed by Bates (1947) and by Green and Weber (1950), is defined as the ratio of the value of the radial integral to its positive or negative part, whichever is larger. As such, it is a measure of the sensitivity of the radial integral calculation to small changes in the wave functions. The value unity indicates that the \( f \)-value is not excessively sensitive to small changes in the wave function.

As Green and Weber have noted, the better agreement of the two methods which is obtained when the theoretical energies are used is indicative only of the numerical accuracy of the work rather than an exact solution to the true Schrödinger equation. However, their opinion was that the oscillator strengths derived from calculated energies were the better values.
Fig. 2.—Abbreviated energy-level diagram

Fig. 3.—Potential and wave functions
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Fig. 1.—Ultraviolet spectrogram showing 3s3p^2 1S_0 → 3s3p^2 3P_1/2, 1/2 transition (McAllister 1959)