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Oscillator Strengths for Ultraviolet Atomic Transitions
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UNDER THE ULTRAVIOLET, VISIBLE, AND
GRAVITATIONAL ASTROPHYSICS RESEARCH PROGRAM:
OSCILLATOR STRENGTHS FOR ULTRAVIOLET ATOMIC
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I. Introduction

The conditions within astrophysical environments can be derived from observational data on atomic and molecular lines. For instance, the density and temperature of the gas are obtained from relative populations among energy levels. Information on populations comes about only when the correspondence between line strength and abundance is well determined. The conversion from line strength to abundance involves knowledge of meanlives and oscillator strengths. For many ultraviolet atomic transitions, unfortunately, the necessary data are either relatively imprecise or not available.

Because of the need for more and better atomic oscillator strengths, our program was initiated. Through beam-foil spectroscopy, meanlives of ultraviolet atomic transitions are studied. In this technique, a nearly isotopically pure ion beam of the desired element is accelerated. The beam passes through a thin carbon foil ($2 \mu\text{g}/\text{cm}^2$), where neutralization, ionization, and excitation take place. The dominant process depends on the energy of the beam. Upon exiting the foil, the decay of excited states is monitored via single-photon-counting techniques. The resulting decay curve yields a meanlife. The oscillator strength is easily obtained from the meanlife when no other decay channels are present. When other channels are present, additional measurements or theoretical calculations are performed in order to extract an oscillator strength. During the past year, three atomic systems have been studied experimentally and/or theoretically; they are Ar I, Cl I, and N II. The results for the first two are important for studies of interstellar space, while the work on N II bears on processes occurring in planetary atmospheres.

II. Accomplishments

(i) Ar I

The resonance lines of Ar I at 1048 and 1067 Å provide the basis of our knowledge of argon in interstellar space. The resonance lines involve the transitions $3p^6-3p^54s[3/2]_1$ and $3p^6-3p^54s[1/2]_1$, respectively. Until now, however, the available data on oscillator strengths for these transitions span an uncomfortably large range (Morton 1991). We have measured a value of 1.92 ± 0.08 ns for the meanlife of the 1048 Å line. This is the most precisely determined f-value for this line and it falls in the middle of the range of previously available results. Cascades into the upper state of Ar I λ 1067 prevented our experimentally determining a meanlife for this transition. However, using the singlet-triplet mixing-angle formulation developed by Curtis (1989; 1991), a collaborator in this program, we extracted a reliable lifetime for λ 1067 as well. The value is 7.96 ± 0.33 ns. The corresponding oscillator strengths are $f(1048) = 0.257 \pm 0.013$ and $f(1067) = 0.064 \pm 0.003$.

These oscillator strengths are within about 10% of the ones used by York and Kinahan (1979) and York (1983), who studied interstellar matter in the solar neighborhood, but the key point is that our results are more precise. Thus the conclusions reached by York and collaborators for α Vir and λ Sco are strengthened. In particular, the argon abundance, like the abundances of nitrogen and oxygen, is approximately solar. As a result, a solar abundance for sulfur is also expected, but since the sulfur abundance appears larger than solar, contamination from S II associated with H II regions is likely affecting the determination of the sulfur abundance. Moreover, our results firmly establish the fact there is a trend of decreasing absorption line width with

increasing atomic mass. The line widths indicate a temperature of about 10^4 K for the neutral gas toward the two lightly reddened stars. This warm, neutral gas appears in clumps of approximately 1 pc in size and thus represents only a small fraction of the volume along the line of sight. Most of the interstellar material then is hot gas associated with the Local Bubble in which the Sun is immersed.

A description of this work was recently submitted to the *Astrophysical Journal* as a collaborative effort with Don York of the University of Chicago. The title page and abstract are included in the Appendix. An abstract for a poster paper describing the meanlife determinations to be presented at the forthcoming annual meeting of the Division of Atomic, Molecular, and Optical Physics of the American Physical Society (DAMOP) is also in the Appendix.

(ii) Cl I

The 1088 and 1097 Å lines of Cl I were studied because recent theoretical results are in conflict with oscillator strengths derived from astronomical data. The astronomical data (Jura and York 1978; Federman 1986) indicate that the 1088 Å line is the stronger of the two, while the theoretical work (Ojha and Hibbert 1990) suggests the converse. *Ab initio* calculations were performed by us to examine possible causes for the discrepancies, but the complexity of this atomic system led to the conclusion that experimental data are needed to resolve the issue, as was also suggested by Keenan and Dufton (1990).

We carefully examined the low energy beam-foil spectrum of Cl in the wavelength range 1078 - 1112 Å by superposing many wavelength scans, each measured with a different foil. The spectral line at 1088.06 Å is identified with the transition to ground from the level described in LS coupling as

$3p^4(^3P)3d^2F_{5/2}$ (Radziemski and Kaufman 1969). The line is a very prominent feature of the spectrum and is unblended. Decay curves for this transition were measured at beam energies of both 130 keV and 170 keV, and a meanlife of 3.3 ± 0.3 ns resulted.

On the other hand, the line at 1097.37 Å, due to the transition between ground and the level described as $3p^4(^3P)3d^2D_{5/2}$ (Radziemski and Kaufman 1969) is very weak; while clearly present, the line appears only as a shoulder on the stronger transition at 1098.07 Å. We measured the ratio of the intensities for these two lines, $R(1088/1097)$, at a number of foil positions, corresponding to times after excitation of 0.4, 2.0, 4.0, 5.5, 7.0, and 9.5 ns. Extrapolation to $t=0$ gives a value for this ratio as the Cl atoms exit the foil of $R = 9.3 \pm 1.1$.

This ratio can be expressed by a product of the ratios of the respective transition probabilities and of the respective excited state populations as the atoms emerge from the foil:

$$R = \frac{A(3d^2F_{5/2} \rightarrow 2P_{3/2})}{A(3d^2D_{5/2} \rightarrow 2P_{3/2})} \frac{N_o(3d^2F_{5/2})}{N_o(3d^2D_{5/2})}$$

A plausible assumption is that the foil excitation mechanism would populate these excited states nearly equally. Together with the equal statistical weights, this leads one to conclude from the large value of R that $f(1088) \gg f(1097)$. Should the levels be *exactly* equally populated initially, the resulting meanlife of the $^2D_{5/2}$ level would be 31 ± 5 ns. That this is plausible is shown by considering the intensity of the λ 1097 line as a function of time after excitation and comparing observations with an assumed

single exponential decay of meanlife 31 ns normalized to the data; agreement obtained is quite good, thus qualitatively confirming the assumption about the excitation process. Were the meanlife to have been only 3ns, the agreement obtained would be much less satisfactory.

For single channel decay, these experimental meanlives correspond to oscillator strengths with values of $f(1088) = 0.081 \pm 0.007$ and $f(1097) = 0.0090 \pm 0.0015$. For comparison, the respective oscillator strengths determined theoretically by Ojha and Hibbert (1990) are 0.016 ± 0.004 and 0.042 ± 0.010 , while the astronomically derived values are $f(1088) = 0.040 \pm 0.010$ (Federman 1986) and $f(1097) = 0.014 \pm 0.005$ (Jura and York 1978). The theoretical work clearly has the strengths reversed; our results confirm the trend seen astronomically, but the experimental and astronomical values for λ 1088 differ at the 3σ level. Since the astronomical result was tied to the somewhat uncertain oscillator strength for λ 1347, we are attempting to remeasure the meanlife and f-value for λ 1347 to see whether or not the differences may be due to normalization.

(iii) N II

For light atoms and singly charged ions, intercombination (spin-changing) lines are very weak, usually several orders of magnitude weaker than allowed transitions under LS coupling. Tripp et al. (1991) recently called attention to an exception in the N II spectrum, where an intercombination line at 748 Å ($2p^2 \ ^1D_2 - 2p3s \ ^3P_1$) is comparable in strength to the allowed decays of 3P_1 . These authors found the 748 Å branching ratio to be about 30% (0.29 ± 0.15) and emphasized the significance of this fact for the modeling of plasmas such as the upper atmospheres of Earth and Titan. They also pointed out that this

effect was predicted by the extensive calculation of carbon sequence oscillator strengths by Fawcett (1987), and suggested that other predictions of that calculation should be tested. If such strong intercombination lines should be at all common in the extreme UV, the consequences for plasma modeling would be important indeed.

We are investigating the following questions with this point in mind. Why is the 748 Å line in N II so strong, and can the same mechanism be expected to act in other important cases? Can semi-empirical calculations making use of existing theoretical and experimental results improve our knowledge of the oscillator strengths for these N II transitions? Can new *ab initio* theoretical calculations give better results for N II, and also for C I and O III?

With regard to the first question, the unusual situation in N II 2p3s is caused by configuration interaction (CI) with the "plunging" configuration 2s2p³, which is higher in energy for C I but lower for large Z. In N II the 2p3s ¹P and ³P are pushed together by CI with the corresponding levels of 2p³. (The 2p³ ¹P is above 2p3s while the 2p³ ³P is below.) Because they are so close in energy, the 2p3s ¹P₁ and ³P₁ mix with each other, causing both to have strong intercombination lines. This effect can be predicted easily: levels of different S but the same J and parity will mix when they are nearby in energy.

There is a second reason why the N II 748 Å line is so strong. The CI with 2s2p³ enhances the 747 Å ¹D-¹P transition at the expense of the ¹S-¹P transition; the interference produced in the dipole integral by the 2p³ component of the 2p3s wavefunction is constructive for the former and destructive for the latter. This provides a further enhancement of the ¹D-³P intercombination line, since it proceeds through the singlet component of the ³P wavefunction and is proportional to the same ¹D-¹P dipole integral. Such

effects are not easy to compute quantitatively with *ab initio* calculations. A powerful method is that used by Fawcett (1987), which begins with Hartree-Fock, includes configuration interaction and relativity, and makes adjustments to fit observed energy levels. The results of such calculations are very valuable in calling attention to unusual effects, such as in the present case, but should be checked whenever possible because the semi-empirical adjustments are not always unique.

In addressing the second question, for simple cases such as this one, the spin-orbit mixing can be determined quite well directly from the observed energy levels. Curtis (1989, 1991) showed the effectiveness of this approach. Published results of two convincing *ab initio* calculations agree that the oscillator strength in pure LS coupling is $0.200 \pm 5\%$ (Beck and Nicolaides 1976; Luo and Pradhan 1989). From the empirically determined spin-orbit mixing we get an oscillator strength for the 1D_2 - 3P_1 transition of $f(^1D_2$ - $^3P_1) = 0.023$.

Alternatively we could start from experiment instead of theory. Baudinet-Robinet et al. (1990) measured a precise meanlife of 0.267 ± 0.010 ns for the $2p3s$ 1P_1 level. A theoretical branching ratio $R = A(747)/A(\text{tot})$ is required to convert this into an f value, but since R is large, the conversion is not very sensitive to it. (Fawcett (1987) gives $R=0.933$; Luo and Pradhan (1989) give $R=0.952$.) The results are $f(^1D_2$ - $^1P_1) = 0.177$ and $f(^1D_2$ - $^3P_1) = 0.023$.

We can apply the same method to the other $2p^2$ - $2p3s$ transitions, but we have less extensive and precise data from which to work. We need the oscillator strengths for pure LS coupling for the multiplets 1S - 1P and 3P - 3P . Taking these from Luo and Pradhan (1989), we get the results shown below. Because we have consistent input data from several convincing sources for the

747 and 748 Å lines, we list their precision at 5%. This is not true for the other lines; we estimate their precision at 50%. We add the results of Fawcett (1987) for comparison in the following table.

LINE	WAVELENGTH	gf(THIS WORK)	gf(Fawcett)
$^1D_2 - ^1P_1$	746.98	0.885	0.943
$^1D_2 - ^3P_1$	748.36	0.115	0.121
$^1S_0 - ^1P_1$	858.35	0.014	0.042
$^1S_0 - ^3P_1$	860.19	0.002	0.005
$^3P_2 - ^3P_1$	672.00	0.097	0.102
$^3P_2 - ^1P_1$	670.88	0.011	0.011
$^3P_1 - ^3P_1$	671.63	0.058	0.059
$^3P_1 - ^1P_1$	670.51	0.007	0.008
$^3P_0 - ^3P_1$	671.41	0.078	0.080
$^3P_0 - ^1P_1$	670.29	0.009	0.010

Except for the transitions involving 1S_0 , where the CI cancellation effect mentioned above makes precision difficult, the agreement with Fawcett (1987) is remarkable. From these results, we predict the branching ratio for λ 748 to be 28%, in agreement with Tripp et al. (1991). A paper describing these results is in preparation.

As for the third question, work is in progress. We are performing *ab initio* calculations on the relevant configurations in the carbon isoelectronic sequence using a variety of well-known programs, including MCHF (Fischer 1978),

MCDF (Dyall et al. 1989), and HFR (Cowan 1981). This work will also be presented as a poster at the DAMOP meeting in May; the abstract appears in the Appendix.

III. Summary

Oscillator strengths for Ar I, Cl I, and N II have been obtained. Our results for Ar I $\lambda\lambda$ 1048, 1067, which are the most accurate to date, are $f(1048) = 0.257 \pm 0.013$ and $f(1067) = 0.064 \pm 0.003$. The improved accuracy strengthens the conclusions of York and collaborators regarding the properties of the interstellar medium toward λ Sco and α Vir. We have completed the first reported laboratory measurements of the oscillator strengths for the Cl I lines at 1088 and 1097 Å; our results are $f(1088) = 0.081 \pm 0.007$ and $f(1097) = 0.0090 \pm 0.0015$. The fact that λ 1088 is the stronger line confirms the prediction derived from astronomical data, contrary to recent theoretical results. In the spectrum of N II, we have used a semiempirical treatment of spin-orbit interaction, in combination with *ab initio* theory, to derive oscillator strengths for UV transitions. Our results confirm and explain the unusual strength of the intercombination line at 748 Å, for which we report $gf = 0.115 \pm 0.006$. With this understanding, the plasma processes associated with planetary atmospheres can be studied with more confidence.

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Appendix

Accurate Oscillator Strengths for Ultraviolet Lines of Ar I: Implications for Interstellar Gas Temperatures

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Abstract

Analysis of absorption from interstellar Ar I in lightly reddened lines of sight provides information on the warm and hot phases of the interstellar medium. The details of the analysis are limited by the quality of the atomic data. Accurate oscillator strengths for the Ar I lines at 1048 and 1067 Å and the astrophysical implications are presented. From lifetimes measured with beam-foil spectroscopy, an f-value for $\lambda 1048$ of 0.257 ± 0.013 is obtained. Through the use of a semi-empirical formalism for treating singlet-triplet mixing, an oscillator strength of 0.064 ± 0.003 is derived for $\lambda 1067$. Because of the accuracy for these new results, the conclusions of York and colleagues from spectra taken with the *Copernicus* satellite are strengthened. In particular, for interstellar gas in the solar neighborhood, argon has a solar abundance and the warm, neutral gas is not pervasive.

Abstract Submitted
for the 1992 Annual Meeting
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Atomic, Molecular and
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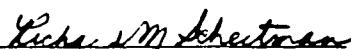
Suggested Poster
Session:
ATOMIC & MOLECULAR
STRUCTURE

PACS Number: 32.70 Fw

Redetermination of the Meanlives of the $3p^5 4s$ $J=1$ Levels of Neutral Argon for the Investigation of Interstellar Matter, R.M. SCHECTMAN, S.R. FEDERMAN and D.J. BEIDECK, Univ. of Toledo*. -To study the structure of nearby interstellar matter, we have re-examined the meanlives of the $3p^5 4s [3/2]_1$ and $[1/2]_1$ levels of neutral argon to determine f -values for the ground state transitions at 1048.2 and 1066.7Å. We measured the meanlife of the $[3/2]$ transition by beam foil techniques. The value 1.92 ± 0.08 ns was obtained. For the $[1/2]$ transition a value was derived from the $[3/2]$ measurement by using experimental term values for the four levels of the $3p^5 4s$ configuration to compute the degree of mixing of the 1P and 3P levels; from the mixing, the ratio of the meanlives of the $[1/2]$ and $[3/2]$ levels can be computed. The value obtained for $[1/2]_1$ was 7.96 ± 0.33 ns. Corresponding f -values were 0.257 ± 0.013 and 0.064 ± 0.003 . Our results agree well with the weighted mean of previous measurements and with theory, but are of increased precision. They will be used to reinterpret Copernicus Satellite Data for neutral argon in the solar neighborhood.

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(x) Prefer POSTER Session


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Abstract Submitted
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Suggested session:
Atomic Spectroscopy (UV)

PACS number: 31

Calculation of UV Oscillator Strengths in N II Using MCHF Wavefunctions. * D.G. ELLIS, *The University of Toledo*. -- Oscillator strengths have been calculated for the ultraviolet transition array $2p^2 - 2p3s$ in the spectrum N II. Recent astrophysical,¹ experimental,² and theoretical³ works have called attention to two interesting features of these lines. First, the intercombination line, $^1D_2 - ^3P_1$, is exceptionally strong; second, the 1P branching ratio $A(^1D-^1P)/A(^1S-^1P)$, is unusually large. Both these effects reflect the strong interaction of $2s^2 2p3s$ with $2s2p^3$; the 1P terms of these configurations cross between N II and O III, while the 3P cross between C I and N II. In the present work, two different sets of Multiconfiguration Hartree-Fock⁴ solutions have been obtained for these states. (One solution set employs multiple orbitals of the same type and the other does not.) These wavefunctions have been used to compute oscillator strengths for all the lines in the $2p^2 - 2p3s$ transition array; the results are compared with published theoretical and experimental values.

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1 T.M. Tripp et al., *ApJ*, 368, 641 (1991)

2 Y. Baudinet-Robinet et al. *Phys.Rev.* 42, 1080 (1990)

3 B.C. Fawcett, *At.Dat.Nuc.Dat.Tables* 37, 411 (1987)

4 C.F. Fischer, *Comp.Phys.Comm.* 1, 151 (1969); 14, 145 (1978)

Prefer poster session



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