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MAGNETIC DIPOLE LINES IN THE $3s^2 3p^x$ CONFIGURATIONS OF ELEMENTS FROM COPPER TO MOLYBDENUM

B. Denne, E. Hinnov, S. Suckewer, S. Cohen

Plasma Physics Laboratory, Princeton University

Princeton, New Jersey 08544

ABSTRACT

A number of spectrum lines arising from magnetic dipole transitions in the $3s^2 3p^5$, $3s^2 3p^4$, $3s^2 3p^3$, $3s^2 3p^2$, $3s^2 3p$, and 3s3p electron configurations in elements $29 \leq Z \leq 42$ have been identified. The lines were observed in the PLT tokamak discharges into which the appropriate elements were introduced by means of laser blowoff. The identifications are based on time- and space-dependence of the observed emissivities, and the systematic consistency of the observed wavelengths with isoelectronic extrapolations based on known lower-Z elements.

I. INTRODUCTION

The energy level structure of the $3s^2 3p^x$ configurations (i.e., the chlorine, sulfur, phosphorus, silicon, and aluminum isoelectronic sequences) are fairly adequately determined for elements up to nickel (Z=28), largely as a result of solar coronal observations and the analysis of Edlén[1] and his co-workers. These energy levels are tabulated in National Bureau of Standards compilations.[2] Empirically adjusted analytical expressions have been developed[3,4] that allow accurate interpolations for any elements that have not been observed directly. However, there are practically no experimental data for the heavier elements because of their low abundances in solar spectra and the difficulties of observing the relatively weak radiative transitions in the high-density, short-duration discharges of many laboratory plasmas.

But it is precisely in the range of elements, about $29 \leq Z \leq 42$, where the magnetic dipole transitions within these configurations become sufficiently intense to be of major interest for localized spectroscopic diagnostics in tokamak-type discharges. The reasons for this, both physical and technical, have been described elsewhere[5-7] together with references to actual applications. In the present paper we shall discuss recent identifications of such magnetic dipole transitions observed in PLT tokamak discharges and, with a few exceptions, not previously published.

The identification, as in the case of the n=2 shell transitions,[6] is based on time- and space-distribution measurements and absolute intensities, all in comparison with known resonance lines of neighboring states, e.g., the 3s-3p and $3s^2\ {}^1S\text{-}3s3p\ {}^1P$ transitions in sodium and magnesium sequences, respectively, and for the heavier elements, the analogous n=4 transitions. The expected approximate wavelengths are predicted from isoelectronic extrapolations of empirical fits in lighter elements or from theoretical

calculations.[4,8,9] There are practically no experimental data for these elements except for a few concurrent measurements.[10-12]

The wavelength measurement accuracy is generally ± 0.3Å or better, the limiting factor being the reliability of interpolation of the spectrometer drive between known reference lines. In a few cases, when a good reference line is in the immediate vicinity, the accuracy is significantly better and is so indicated. On the other hand, if the lines overlap with the relatively abundant carbon or oxygen ion lines, or, even worse, with higher grating-order wavelengths of strong resonance lines of lower ionization states of the element under investigation, the measurement accuracy is less. In the latter case, it is often not possible to establish adequately the time- and space-dependence of the line under investigation, and such identifications are regarded as tentative. For confirmation it is then necessary to establish isoelectronic interpolations with neighboring elements. Such lines, with substantial inherent interference from o .er lines, are not useful for plasma diagnostics, but they are nevertheless needed for establishing confidence in the identifications along the sequences. According to the usual convention, wavelengths above 2000Å are given in air.

II. RESULTS

Tables I-IV present the results of the wavelength measurements. There are three types of entries:

1) The numbers without brackets indicate wavelengths, in Ångstroms, where we consider the indicated transitions reliably established.

2) In many cases, especially those of weaker lines, the time- and space-dependence of the emissivity cannot be adequately established. Such tentative identifications are indicated with square brackets.

3) The numbers in parentheses give interpolated values based on measured wavelengths in the same column as a guide for future measurements.

In general, the facility of measurements and reliability of interpretations are greatest for the simple configurations at the ends of the period, shown in Table I. However, the quality of the results deteriorates for the more intricate configurations given in subsequent tables.

The measurements have been performed only with copper, germanium, selenium, zirconium, and molybdenum, mostly because of the scarcity of available experimental time on the PLT tokamak. Also, because of spectrometer sensitivity limitations, there have been no measurements of weak line intensities in the 1000-1400Å interval.

A. Magnesium Sequence, 3s3p Configuration

The $^3P_2$ - $^3P_1$ transition wavelengths of this configuration are given in the first column of Table I. The copper, germanium, selenium, zirconium, and molybdenum wavelengths are measured; the others interpolated. The interpolated wavelengths should be accurate to better than ± 1Å, and of course these data allow interpolation to the other intervening elements with comparable accuracy. The transition energies are slightly larger than the calculated values,[8] with the deviation increasing slowly with the atomic number, Z.

Unlike the other configurations discussed in this paper, the 3s3p is not the ground configuration of the magnesium sequence. Nevertheless the $^2P_2$ - $^2P_1$ lines are fairly bright, consistent with the observations[13,14] of the $3s^2\ ^1S_o$ - $3s3p^3P_1$ intercombination line brightnesses, and therefore very useful for spectroscopic plasma diagnostics.

There do not appear to be any published experimental observations of this transition[15] beyond the coronal line of FeXV at 7058.6Å. However, the GeXXI line has recently been identified in the Doublet III spectra by Burrell and Groebner,[10] in very good agreement with our result.

B. Aluminum Sequence, $3s^23p$ Configuration

The second column in Table I gives the wavelengths of the $^2P_{3/2}$-$^2P_{1/2}$ transitions, again with the interpolated values in parentheses. In this case, extrapolation of the empirically adjusted (for $Z \leq 28$) formulas given by Smitt et al.,[4] systematically give slightly larger transition energies, e.g., λ = 486.4Å for MoXXX.

C. The Chlorine Sequence, $3s^23p^5$ Configuration

The $^2P_{1/2}$-$^2P_{3/2}$ transition wavelengths are given in the last column of Table I. These transition energies follow quite closely isoelectronic extrapolations of the semiempirical formulas given by Svensson[3] and also (within a constant factor) of the Dirac-Fock energies of Kim and Huang,[9] who have calculated the radiative transition rates for these ions.

D. The Sulfur Sequence, $3s^2 3p^4$ Configuration

In the $3s^2 3p^4$ configuration there are five magnetic dipole lines, but two of those, the $^1D_2 - {}^3P_1$ and $^3P_1 - {}^3P_0$ are expected to be weak because the radiative branching strongly favors the other component, $^1D_2 - {}^3P_2$ and $^3P_1 - {}^3P_2$, respectively. In Table II, the measured wavelengths of these weak transitions are all in the tentative category. However, the stronger lines in Zr XXV and MoXXVII are quite well established, and are sufficient to determine the energy separations of all levels except the $^3P_0$, which needs further confirmation. There have been some difficulties in determining the $^1S_0 - {}^3P_1$ transition in selenium and germanium although the line appears quite strong in zirconium and molybdenum - the uncertainty in the latter case is due to strong interfering radiation, rather than a weakness of the line.

In spite of the weakness of the $^1D_2 - {}^3P_1$ and $^3P_1 - {}^3P_0$ sequence lines, they are of special interest in plasma diagnostics because of their relatively long wavelengths and their potential usefulness for spectrometer sensitivity calibration by means of radiative branching ratios. It is therefore important to establish their wavelengths and relative intensities directly, even in cases where the stronger lines of the same configuration may be more appropriate for many diagnostic purposes.

Isoelectronic extrapolations from the lower-Z data[4] tend to give systematically slightly larger energy separations than the experimental observations.

E. The Silicon Sequence, $3s^2 3p^2$ Configuration

The measured wavelengths in the $3s^2 3p^2$ configuration are given in Table III. The ^3P levels, and to a lesser extent the $^1S_0$ level, are fairly well established, but so far we have not located the transitions from the $^1D_2$ level, except for a cursory observation of the $^1D_2 - {}^3P_2$ transition in Cu and Ge. This is not because of any known inherent difficulty, but rather the scarcity of experimental time on PLT. The comment about radiative branching ratios for intensity calibration also applies to the transitions from the $^1D_2$ level in this sequence.

In this configuration, the isoelectronic extrapolation, from $Z \leq 28$, predicts an energy separation slightly too small for the $^3P_2 - {}^3P_1$, and too large for the $^3P_1 - {}^3P_0$ and $^1S_0 - {}^3P_1$ levels.

F. The Phosphorus Sequence, $3s^2 3p^3$ Configuration

There has been a notable lack of success in identifying lines in this configuration. There are no adequate theoretical predictions of either the energy levels or the radiative transition rates, and the isoelectronic extrapolations are likely to be more precarious than in the sulfur or silicon sequences.

As a result, all the lines shown in Table IV are rather tentative identifications and require further confirmation. All these lines are weak. Thus the lines assigned to the $^2D_{3/2} - {}^4S_{3/2}$ transition are some 3-5 times less intense than the neighboring $^3P_1 - {}^3P_0$ lines of the silicon sequence. Furthermore, in several cases, adjacent strong OIII and OIV resonance lines prevent adequate measurement of both spectral intensity distribution and time behavior of these lines (increasing the amount of injected element can change the target plasma properties including the time behavior of the oxygen lines).

Of the lines shown in Table IV, we presently have the most confidence in the lines ascribed to the $^2D_{5/2} - {}^2D_{3/2}$ transition. Although weak, these lines have no interfering plasma background lines in their vicinity. They will be of substantial interest for plasma diagnostics if the identifications are confirmed.

III. DISCUSSION OF THE RESULTS

It appears from the data that the energy level separations corresponding to the lines in Table I are well-established up to molybdenum, and could be extrapolated slightly beyond, perhaps to Z = 45-48. All these lines are quite strong and well-suited for a variety of spectroscopic plasma diagnostics. However, for interpretation of measured local emissivities in terms of corresponding ion densities, a considerable amount of work is still required. In particular, the strength of the $3s3p\ {}^3P_2-{}^3P_1$ line relative to the $3s^2-3s3p$ resonance ($^1S_0 - {}^1P_1$) line and intercombination ($^1S_0 - {}^3P_1$) line requires quantitative interpretation, both experimentally and theoretically. For this purpose, it would be important to measure simultaneously the emissivities of the three lines for different elements and at different electron densities.

In the sulfur and silicon sequences considerable details are still missing or in need of confirmation; and in the phosphorus sequence the work is only beginning. The lines in these sequences are weaker and hence more difficult to measure quantitatively. But because of their greater variety, especially in the wavelength range, these lines offer a correspondingly greater versatility for potential diagnostic application.

Recently, detailed radiative transition rates have been calculated for the $2s^22p^x$ configurations by Cheng, Kim, and Desclaux,[16] and the expected

steady-state population densities in plasmas of different electron density by Feldman, Doschek, and Bhatia.[17] Similar calculations for the n=3 configurations would be very valuable for further investigation of these energy levels and for quantitative diagnostic applications, particularly for the phosphorus sequence ions.

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Table I

Wavelengths (Å) of the Indicated Transitions in the Magnesium, Aluminum, and Chlorine Sequences.(*)

Z	$3s3p\ ^3P_2 - {}^3P_1$	$3s^23p\ ^2P_{3/2} - {}^2P_{1/2}$	$3s^23p^5\ ^2P_{1/2} - {}^2P_{3/2}$
29 Cu	3941.6	3007.6 ± 0.2	3500.4
30 Zn	(3296.8)	(2532.0)	(2924.0)
31 Ga	(2775.4)	(2146.7)	(2459.6)
32 Ge	2350.2	1832.7	2085.1 ± 0.1
33 As	(2001.7)	(1573.1)	(1780.0)
34 Se	1714.1	(1358)	1527.8
36 Kr	(1275)	(1027)	(1145)
38 Sr	(965)	(791)	(875)
40 Zr	741.5	618.5	679.1
41 Nb	(653.3)	(549.7)	(601.7)
42 Mo	577.5	490.1	534.9

*Numbers in parentheses are interpolated wavelengths. Measurement uncertainties are ± 0.3Å unless stated otherwise.

Table II

Wavelengths in the $3s^2 3p^4$ Configuration of the Sulfur Sequence.(*)

Z	$^3P_1 - {}^3P_2$	$^3P_1 - {}^3P_0$	$^1D_2 - {}^3P_2$	$^1D_2 - {}^3P_1$	$^1S_0 - {}^3P_1$
29 Cu	[4193.6]		(1906)	(3492)	(1190)
32 Ge	2406.9		(1361)	[3131.3]	[952.9]
34 Se	1727.7	[5645.0]	(1088)	[2935.8]	[808.8]
36 Kr	(1271)	(3105)	(871.1)	(2767)	(680)
38 Sr	(956)		(700.0)	(2610)	
40 Zr	731.8 + 0.2	(1274)	564.9	[2476]	474.2
42 Mo	569.8 ± 0.1	[889.2]	458.6 ± 0.2	(2348)	[395.7]

*Numbers in square brackets are tentative identifications. In the interpolations (values in parentheses) it is assumed that the tentative identifications are correct.

Table III

Wavelengths in the $3s^2 3p^2$ Configuration of the Silicon Sequence.(*)

Z	$^3P_1 - {}^3P_0$	$^3P_2 - {}^3P_1$	$^1D_2 - {}^3P_2$	$^1D_2 - {}^3P_1$	$^1S_0 - {}^3P_1$
29 Cu	5375.8	(7105)	[2529.7]	(1871)	952.8
32 Ge	2933.7 ± 0.2	5170.3	[1810.4]	(1341)	754.1
34 Se	2042.0	4396.5	(1413)	(1069)	[639.6]
36 Kr	(1463)	(3840)	(1097)	(854)	(541)
40 Zr	807.4	3101.3	(669)	(550)	(385)
42 Mo	618.5	2841.1 ± 0.2	(527)	(445)	[325.3]

*See footnote for Table II.

Table IV

Wavelengths in the $3s^2 3p^3$ Configuratior of the Phosphorus Sequence.(*)

Z	$^3D_{3/2} - {}^4S_{3/2}$	$^2D_{5/2} - {}^2D_{3/2}$	$^2P_{3/2} - {}^4S_{3/2}$	$^2P_{1/2} - {}^4S_{3/2}$
29 Cu	[2085.3]		[944.2]	
32 Ge	[1779]	[5702.3]	[703.6]	[894.8]
34 Se	[1534]	4276.0	(569.2)	
40 Zr	(787)	2549.8		
42 Mo	[609.8]	2285.4 ± 0.1		

*See footnote for Table II.