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SPECTROMETER SENSITIVITY CALIBRATION IN THE EXTREME UV BY MEANS OF BRANCHING RATIOS OF MAGNETIC DIPOLE LINES

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ABSTRACT

Relative intensity measurements of various line pairs resulting from magnetic dipole transitions within the configurations s^2p^2 and s^2p^4, in conjunction with calculated transition probabilities, have been used to determine the wavelengtn dependence of the sensitivity of a grazing incidence spectrometer, in the range 400-1000 Å. Emissions from Cr XIX, Fe XXI, Ni XXI and XXIII, Cu XXIV, and Zr XXVII ions in PLT tokamak discharges were used for this purpose. Absolute sensitivity of the spectrometer at selected wavelengths had been determined by the traditional hydrogen, helium, carbon, and oxygen electric-dipole line pairs from the same discharges. Similar attempts to use transitions in the s^2p^3 configurations in Cr XVIII, Zr XXVI, and Mo XXVIII ions resulted in significant discrepancies that are ascribed to uncertainties in the corresponding calculated transition probabilities.

I. INTRODUCTION

A measurement of the brightness of two spectrum lines that originate from the same upper level and have a reliably known radiative branching ratio establishes the relative sensitivity of the spectrometer at the two wavelengths. If the sensitivity is known absolutely at one of the wavelengths, e.g., by calibration against a black body, such measurements serve to calibrate the instrument at the other wavelength, where absolute calibration may otherwise be difficult, e.g., in the vacuum UV.

This method of absolute calibration[1] of vacuum-UV spectrometers has the advantage of being done *in situ*, which allows frequent checks of the calibration. However, the number of suitable line pairs is limited, necessitating interpolations over considerable wavelength intervals with concomitant uncertainties.

Figure 1 shows the line pairs used for calibration[2] of a two-channel grazing-incidence spectrometer attached to the PLT tokamak at Princeton. Although in principle many more line pairs are available (an extensive list has been compiled by Wiese and Martin[3]), in practice the choice has been limited to the pairs shown, either because of accidental overlap with other lines in tokamak discharges, or because one or the other of the pair components has been too weak to measure.

Clearly, there are substantial gaps in the curve, particularly in the 600-900 Å and 300-500 Å intervals where the interpolation is quite uncertain. Furthermore, because of the inherent uncertainties both in the calculated transition probabilities and in the brightness measurements, it would be very desirable to have available redundant determinations of the sensitivity curve.

The magnetic dipole lines emitted by transitions between the levels of the ground configurations of highly ionized, medium-Z elements provide the means to complement the sensitivity calibration in the indicated wavelength intervals. Such elements, e.g., iron, titanium, copper, molybdenum, etc., may be present spontaneously as contaminants in high temperature plasma devices, or they may be deliberately added for diagnostic purposes. In this paper we describe attempts to use such magnetic dipole line pairs in the tokamak discharges to improve the sensitivity calibration of the grazing incidence spectrometer, starting essentially from measured calibration points similar to those in Fig. 1.

II. EXPERIMENTAL ARRANGEMENT

The instrument being calibrated is a two-channel Spex 1-m grazing-incidence spectrometer equipped with a 2400 grooves/mm holographically ruled Jobin-Yvon grating with gold coating, at 85° angle of incidence. The detectors are Bendix magnetic electron multipliers with tungsten photocathodes. The nominal wavelength range is from zero-order to 1000 Å with one channel, and from about 300-1250 Å with the other. The spectral band-pass, essentially determined by the slit widths, was 1.2 Å for the lower wavelength and 0.8 Å for the higher wavelength channel.

This spectrometer was attached to the PLT tokamak, and the same view of the plasma was observed with a 1/2 m Ebert-Fastie type Jarrell-Ash mono-chromator, with an effective wavelength range from air cutoff to about 7500 Å. The latter instrument was absolutely calibrated against a standard tungsten ribbon lamp above 2500 Å, and a standard argon mimi-arc[4] in the range 1920-3340 Å.

The calibration points corresponding to those of Fig. 1 were then established as described before.[1,2] Concerning these, we offer the following comments. Clearly, the absolute ordinates of the sensitivity curve depend on incidental conditions such as photomultiplier high voltage, or the spectral bandpass (i.e., slit widths) used. We are thus concerned only with the shape of the sensitivity curve, which is presumably determined by the characteristics of the grating and the photocathode efficiency. In the present case we should expect the sensitivity curves of the two channels to be parallel, although minor deviations could occur as a result of optical alignment errors, or possibly variations of details in the photocathode surfaces.

III. WAVELENGTHS AND TRANSITION PROBABILITIES

In order to investigate the sensitivity behavior in the gaps at ~ 600-900 Å and ~ 300-500 Å (Fig. 1) we have systematically measured the relative intensities of pairs of magnetic dipole lines in the ns^2np^2, ns^2np^4, and ns^2np^3 configurations of chromium, iron, nickel, and copper ions for n=2, and zirconium and molybdenum ions for n=3. The wavelengths of these transitions have been determined recently, mostly for their utility for high temperature plasma diagnostics.[5-7] The radiative transition probabilities have been calculated by Cheng, Kim, and Desclaux[8] for all the n=2 configurations, and by Froese Fischer and Saha[9] for the $2s^22p^4$. For the n=3 configurations, there is a partly empirical calculation by Sugar and Kaufman,[10] and ab initio calculations by Biémont and Bromage[11] for $3s^23p^2$ and Huang[12] for the $3s^23p^3$ configuration. In the cases of overlap there is quite generally a very good agreement between the different calculations.

For our purposes, we require line pairs with one component near a previously established point on the sensitivity curve (or in the range of the directly calibrated 1/2 meter monochromator), and the other in the unknown gap. With sufficient redundancy of such measurements, hopefully a self-consistent curve will emerge that will also allow judgment of the adequacy of the calculated transition probabilities.

We consider calculations of the simpler p^2 and p^4 configurations to be more reliable and attempt to construct the sensitivity curve from these - particularly the $^1D_2 \rightarrow {}^3P_{1,2}$ pairs of the p^2 configuration with calculated branching ratios close to unity. Transitions in the more complicated p^3 configuration - although in principle more versatile and useful - will be treated with more caution, especially in cases where the calculated transition probability is very small.

The appropriate transitions are listed in Tables I and II with the transition rates from the indicated references adjusted to the observed wavelengths by multiplying with $(\lambda^3_{calc}/\lambda^3_{obs})$. The wavelengths of Zr XXVII and Cr XVIII (other than the 793.4 Å line) have not been published before, except in oral presentations at American Physical Society Meetings.

IV. CONSTRUCTION OF THE SENSITIVITY CURVE

The results of the improved calibration procedure are shown in Fig. 2. The starting point, as mentioned above, is the set of line pairs corresponding to those in Fig. 1, solid dots for the low wavelength channel, open circles for the high wavelength channel. (We note that, although the basic instrument is the same as for Fig. 1, quantitative comparisons are not feasible because both the grating and the detectors had to be changed and there were modifications of alignment, slit-widths etc., following a vacuum

accident in 1978). In addition to the absolute sensitivity points, the relative sensitivity of the two channels was measured by successively observing some strong line (e.g., CIII 977 Å, OIV 790 Å, OV 630 Å) in the discharge with both channels. This ratio, shown by crosses(+) in Fig. 2, is more accurate than the individual calibration points, and it serves as a constraint in locating the sensitivity curves of the two channels. However, the reason for the variation of the sensitivity ratio is not known, and it is not safe to extrapolate it much beyond the measured range.

The response of one of the channels to each of the indicated magnetic dipole line pairs was then measured while the other channel was monitoring some other line of the same element for discharge reproducibility. The sensitivity ratio at the two wavelengths is then simply the ratio of the detector responses divided by the appropriate transition probability ratio, from Table I. In each pair the component closer to a measured calibration point (indicated by ▼, ▽ in Fig. 2) was then plotted to a provisional sensitivity curve, and the other component (▲, △) located on the graph. From the latter, crosses (x) indicate the location of the sensitivity of the other channel, according to the above-mentioned ratio. Improved curves were then drawn and the points replotted where necessary with the results shown in Fig. 2.

One of the new points on the higher wavelength channel (□) corresponding to the Ni XXI 779-2818 Å line pair is an absolute measurement, i.e., directly based on the absolutely calibrated 1/2 meter monochromator measurement. There are various other prospects for such absolute measurements both in the s^2p^4 and s^2p^3 configuration. However, the long wavelength component is generally quite weak and so far we have not had sufficiently quantitative results of this type.

The remaining scatter in the data points in Fig. 2, of the order of 20%, appears to be inherent in the measurement uncertainties with our present instrumentation. There is no evidence of systematic deviations that might indicate any problems with the transition probabilities in Table I.

V. THE s^2p^3 CONFIGURATIONS

In the use of the s^2p^3 configurations for improving the calibration, the situation is at present less satisfactory, although in principle this configuration affords greater versatility. As a representative example, the $2s^22p^3$ configuration of Cr XVIII is shown in Fig. 3, with our experimentally determined wavelengths (in Å) and the corresponding energy levels (in cm^{-1}), labelled in the LS coupling notation. The two wavelengths in brackets (deduced from Ritz combination) have not been measured. The 999 Å line is weak and our spectrometer relatively insensitive at this wavelength, and the 879 Å line overlaps with the fairly strong 293.2 Å ($2s2p\ ^3P_1 \rightarrow 2s^2\ ^1S_0$) intercombination line of Cr XXI, in third order. This of course would not prevent its use for normal-incidence spectrometers, where the low wavelength sensitivity is small. (We also note as a curiosity that in the corresponding configuration of FeXX every potentially useful calibration line overlaps with some higher order resonance line of other ionization states).

Even without these two lines, there are evidently line pairs of interest in this configuration not only for relative calibration, but also absolute values, using the 2606 and 4039 Å lines and the transition probabilities listed in Table II.

There is also the prospect of using some line pairs that do not originate from the same level for this purpose. Thus the relatively long-lived ^2D states may be statistically populated, i.e., in the ratio 3:2, by

electron and ion collisions even at fairly low plasma densities, in which case the relative emissivities, e.g., of 793 and 663 Å, are directly comparable. More generally, the relative populations of all the levels of the $2s^2 2p^x$ configurations, and hence the corresponding specific emissivities of the magnetic dipole lines for elements from scandium to krypton, have been calculated by Feldman, Doschek, and Bhatia[13] by means of a detailed collisional-radiative model. Although the calculation involves only approximately known rate coefficients, it should nevertheless give a fairly adequate evaluation of the relative populations, at various plasma conditions of interest.

Nevertheless, in our first attempt to use the Cr XVIII lines for intensity calibration, we experienced difficulties. Firstly, there are some factor-of-two-type discrepancies in the expected relative intensities deduced from the data of Cheng et al.,[8] and Feldman et al.,[13] which make systematic comparisons uncertain. And secondly, we had some difficulties in measuring the 663 Å line and the 2606 Å line brightnesses - the first because of partial overlap with second- and third-order resonance lines of Cr VIII - XII, and the second because of relatively low sensitivity of the 1/2 meter spectrometer at this wavelength. However, some systematic features and discrepancies in these measurements are worth mentioning.

From the data of Feldman et al., it does indeed follow that the relative ^2D level populations of Cr XVIII should be close to statistical at our experimental conditions ($n_e \approx 2.5 \times 10^{13}$ cm^{-3}, $T_e \approx 1$ keV), whereas the $^2P_{1/2}$ and $^2P_{3/2}$ levels are lower by approximately a factor 2 and 3.5-4, respectively. Thus the relative populations of the four excited levels $^2D_{3/2}$: $^2D_{5/2}$:$^2P_{1/2}$:$^2P_{3/2}$ should be about 4:6:1:1, with increasing uncertainties for the last two.

The Feldman predicted ratio of the 793:663 Å line intensities is 12, in good agreement with the ratio deduced from Cheng et al. radiative rates. The experimental value is in the range 9-14, reflecting the uncertainty in the 663 Å line intensity measurement mentioned above, with a most likely value 10 or 11. In this connection we note that the isoelectronic intensity ratio, $^2D_{3/2} + {}^4S_{3/2}/{}^2D_{5/2} + {}^4S_{3/2}$ has also been measured in Ni XXII, Cu XXIII, and Ge XXVI (at 634.8:477.7, 585.0:434.8,427.9:319.1Å, respectively) with the results 4.0, 3.0, 2.4, in quite systematic agreement with Feldman et al. predictions. From this we conclude that at least the relative $^2D_{3/2} + {}^4S_{3/2}/{}^2D_{5/2} + {}^4S_{3/2}$ radiative rates are essentially correct.

However, the measured relative intensity of the 4039 Å line is smaller than predicted (the corresponding ratio, $^2D_{5/2} + {}^2D_{3/2}/ {}^2D_{5/2} + {}^4S_{3/2}$, has not been measured in any other element so far), implying that the calculated radiative rate of $^2D_{5/2} + {}^2D_{3/2}$ is too large by about a factor 1.5 in the Cheng et al. paper, and a factor at least 2 in Feldman et al., relative to the other transitions from the ^2D levels of Cr XVIII.

The entire intensity pattern is shown in Fig. 4, normalized to the strongest, 793 Å line, intensity. For the Cheng et al. rates, we have assumed the relative level populations 4:6:0.67:0.67 which give the best agreement, although the last two are somewhat lower than the values deduced from the density variation in the Feldman paper, as mentioned above. (Also, the Feldman value for the 4039 Å emissivity has been lowered by a factor 1.5 in Fig. 4, as it appears to be plotted incorrectly in their Fig. 5.)

Evidently, there is a fairly good general agreement in the emissivity pattern except for the two long-wavelength lines, which unfortunately are the most interesting for spectrometer calibration purposes. Aside from these, the calculated rate for the 378 Å transition appears too large by at least a

factor 1.5 relative to the others. And the factors used in normalization in Fig. 4 need to be quantitatively investigated.

In Fig. 5, the sensitivity curves of Fig. 2 are reproduced, and the 722 Å and 442 Å lines fitted to the curves. The other points, 793 Å and 378 Å, located according to the emissivities in Feldman et al., then show a substantial agreement for the first, a significant discrepancy for the second. As indicated above, the 663 Å line would fit well on the curve, albeit with fairly large experimental uncertainty, provided that it is located relative to the 793 Å line rather than the 4039 Å line emissivity. Likewise, if we were to use the transition rate in Table II for the 2604 Å line, all the chromium points would be above the curves by about a factor 2 (although the discrepancy would be less if we used the relative emissivities from Feldman et al.). Thus it appears that the p^3 configuration radiative transitions are not yet adequately quantitative for the intensity calibration procedure, at least in Cr XVIII.

The other points in Fig. 5 pertain to relative intensities of transitions from the $^2P_{3/2}$ level of Zr XXVI (triangles) and Mo XXVIII (squares). The measured wavelengths and relative intensities for these $3s^23p^3$ configurations have been published recently.[7] In Fig. 5 the points corresponding to the $^2P_{3/2} + {}^2D_{5/2}$ transition, 582 Å in zirconium, 470 Å in molybdenum, are fitted to the curve, and the other points plotted according to the transition probabilities given in Table II. In the case of molybdenum, the 390 Å line was measured with the lower wavelength channel, and for comparison this point is shifted upward according to the relative channel sensitivity given in Fig. 2. While this shift at 390 Å is somewhat uncertain, it does not change the general picture.

In both cases, the relative transition probability of the $^2P_{3/2} + {}^2D_{3/2}$ transition, as given in Table II, appears too large, in the case of Mo XXVIII by about a factor 4. The relative transition probability of the $^2P_{3/2} + {}^2P_{1/2}$ line in zirconium (846 Å) seems too small by about a factor 1.7. In molybdenum, the corresponding 643 Å point fits exactly on the curve (relative to the 470 Å line), although in view of the relative faintness of the line the measurement uncertainties may make this result partly fortuitous. In either case, the $^2P_{3/2} + {}^4S_{3/2}$ transition (242 Å in the Mo XXVIII, 299 Å in Zr XXVI), expected to be weak,[7,12] was not measured, although this would be clearly of interest. Intensities of lines from other levels of these configurations were measured, but at present there are no quantitative population calculations (comparable to Ref. 13 for the n=2 configurations) for quantitative intercomparisons, and the radiative lifetimes, even of the ^2D levels, are too short to allow invoking relative statistical populations.

VI. CONCLUSIONS

In experiments with high temperature and not very high density plasma devices there exists a large variety of possibilities of extending and improving the line branching ratio method of *in situ* spectrometer sensitivity calibration by utilizing magnetic dipole transitions in highly ionized atoms. Good self-consistent results were obtained, using calculated radiative transition rates for lines in the s^2p^2 and s^2p^4 configurations, in calibrating a spectrometer in the wavelength range 400-1000 Å. However, in the s^2p^3 configurations substantial discrepancies were revealed that apparently indicate difficulties in the transition rate calculations, and will require systematic quantitative investigations, both experimental and theoretical, for their resolution.

ACKNOWLEDGMENTS

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TABLE I

Line Pairs In The s^2p^2 and s^2p^4 Configurations

Spectrum	Transition	λ(Å)	A(sec^{-1})[a]	(Ref.)
Cr XIX	$2s^22p^2(^1D_2 \rightarrow {}^3P_1)$	731.1	5.6×10^3	(C)
	$(^1D_2 \rightarrow {}^3P_2)$	979.1	5.9×10^3	(C)
Fe XXI	$2s^22p^2(^1D_2 \rightarrow {}^3P_1)$	585.8	1.6×10^4	(C)
	$(^1D_2 \rightarrow {}^3P_2)$	786.1	1.5×10^4	(C)
Ni XXIII	$2s^22p^2(^1D_2 \rightarrow {}^3P_1)$	465.4	4.1×10^4	(C)
	$(^1D_2 \rightarrow {}^3P_2)$	614.8	3.7×10^4	(C)
Cu XXIV	$2s^22p^2(^1D_2 \rightarrow {}^3P_1)$	414.1	6.5×10^4	(C)
	$(^1D_2 \rightarrow {}^3P_2)$	540.0	5.8×10^4	(C)
Zr XXVII	$3s^23p^2(^1D_2 \rightarrow {}^3P_1)$	551.5	4.0×10^4	(S)
			3.9×10^4	(B)
	$(^1D_2 \rightarrow {}^3P_2)$	670.8	3.4×10^4	(S)
			3.4×10^4	(B)
Ni XXIII	$2s^22p^4(^3P_1 \rightarrow {}^3P_0)$	2818.2	5.7×10^2	(C)
			5.8×10^2	(F)
	$(^3P_1 \rightarrow {}^3P_2)$	779.5	4.1×10^4	(C)
			4.1×10^4	(F)

[a]Adjusted for observed wavelength.

C : Cheng, Kim, and Desclaux [8]

S : Sugar and Kaufman [10]

B : Biemont and Bromage [11]

F : Froese Fisher and Saha [9]

TABLE II

Transitions in the s^2p^3 Configuration

Spectrum	Transition	λ(Å)	A(sec^{-1})[a]	(Ref.)
Cr XVIII	$2s^22p^3(^2P_{3/2} - {}^2P_{1/2})$	2606.4	3.8×10^2	(C)
	$(^2P_{3/2} - {}^2D_{5/2})$	[879.2]	5.2×10^3	(C)
	$(^2P_{3/2} - {}^2D_{3/2})$	722.1	1.6×10^4	(C)
	$(^2P_{3/2} - {}^4S_{3/2})$	378.0	1.6×10^4	(C)
	$(^2P_{1/2} - {}^2D_{3/2})$	[998.7]	3.3×10^3	(C)
	$(^2P_{1/2} - {}^4S_{3/2})$	442.1	1.3×10^4	(C)
	$(^2D_{5/2} - {}^2D_{3/2})$	4038.6	1.3×10^2	(C)
	$(^2D_{5/2} - {}^4S_{3/2})$	663.1	3.2×10^2	(C)
	$(^2D_{3/2} - {}^4S_{3/2})$	793.4	6.1×10^3	(C)
Zr XXVI	$3s^23p^3(^2P_{3/2} - {}^2P_{1/2})$	846.2	9.2×10^3	(S)
			9.2×10^3	(H)
	$(^2P_{3/2} - {}^2D_{5/2})$	582.3	2.3×10^4	(S)
			2.3×10^4	(H)
	$(^2P_{3/2} - {}^2D_{3/2})$	474.1	1.1×10^5	(S)
			1.1×10^5	(H)
Mo XXVIII	$3s^23p^3(^2P_{3/2} - {}^2P_{1/2})$	643.0	2.1×10^4	(S)
			2.0×10^4	(H)
	$(^2P_{3/2} - {}^2D_{5/2})$	470.0	4.4×10^4	(S)
			4.4×10^4	(H)
	$(^2P_{3/2} - {}^2D_{3/2})$	389.9	2.1×10^5	(S)
			2.1×10^5	(H)

[a]Adjusted for observed wavelength.

C : Cheng, Kim, and Desclaux [8]

S : Sugar and Kaufman [10]

H : Huang [12]

FIGURE CAPTIONS

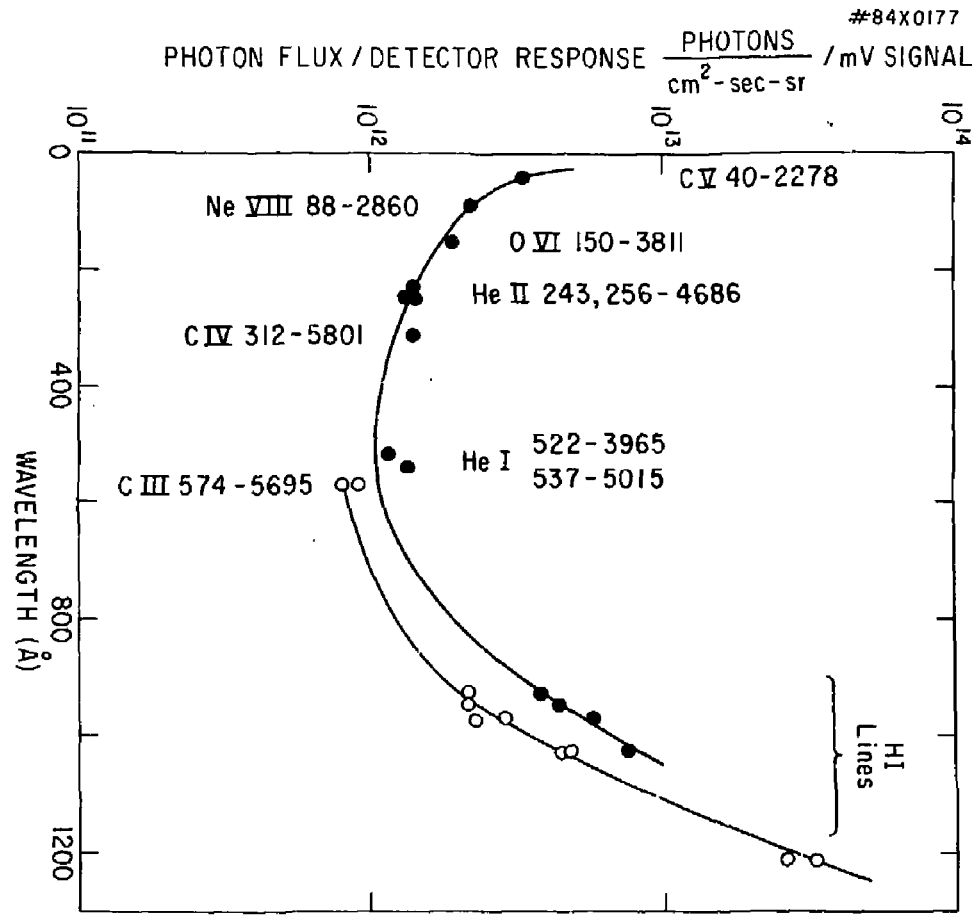
FIG. 1 Reciprocal sensitivity as a function of wavelength for the low wavelength (O) and high wavelength (O) channels of a 1 m grazing-incidence bichromator, from Ref. 2.

FIG. 2 Reciprocal sensitivity curves in the present experiment, supplemented with the branching ratios of indicated magnetic dipole line pairs, and subject to the separately measured channel sensitivity ratio shown at the top.

FIG. 3 Energy level scheme of the $2s^2 2p^3$ configuration of Cr XVIII, constructed from the observed wavelengths (in Å).

FIG. 4 Expected relative intensities of Cr XVIII lines compared with measurements, normalized to the 793 Å line. The relative populations of the $^2D_{3/2}:^2D_{5/2}:^2P_{1/2}:^2P_{3/2}$ levels used in conjunction with Cheng et al. ratios are 4:6:0.67:0.67.

FIG. 5 Sensitivity curves from Fig. 2, with measured line-pair ratios of Cr XVIII (O,O) Zr XXVI (Δ,Δ) and Mo XXVIII (,). The filled symbols are fitted to the curves. The 390Å point of Mo XXVIII is shifted as shown to correspond to the high wavelength channel.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800
1200
WAVELENGTH (Å)
C V 40-2278
Ne VIII 88-2860
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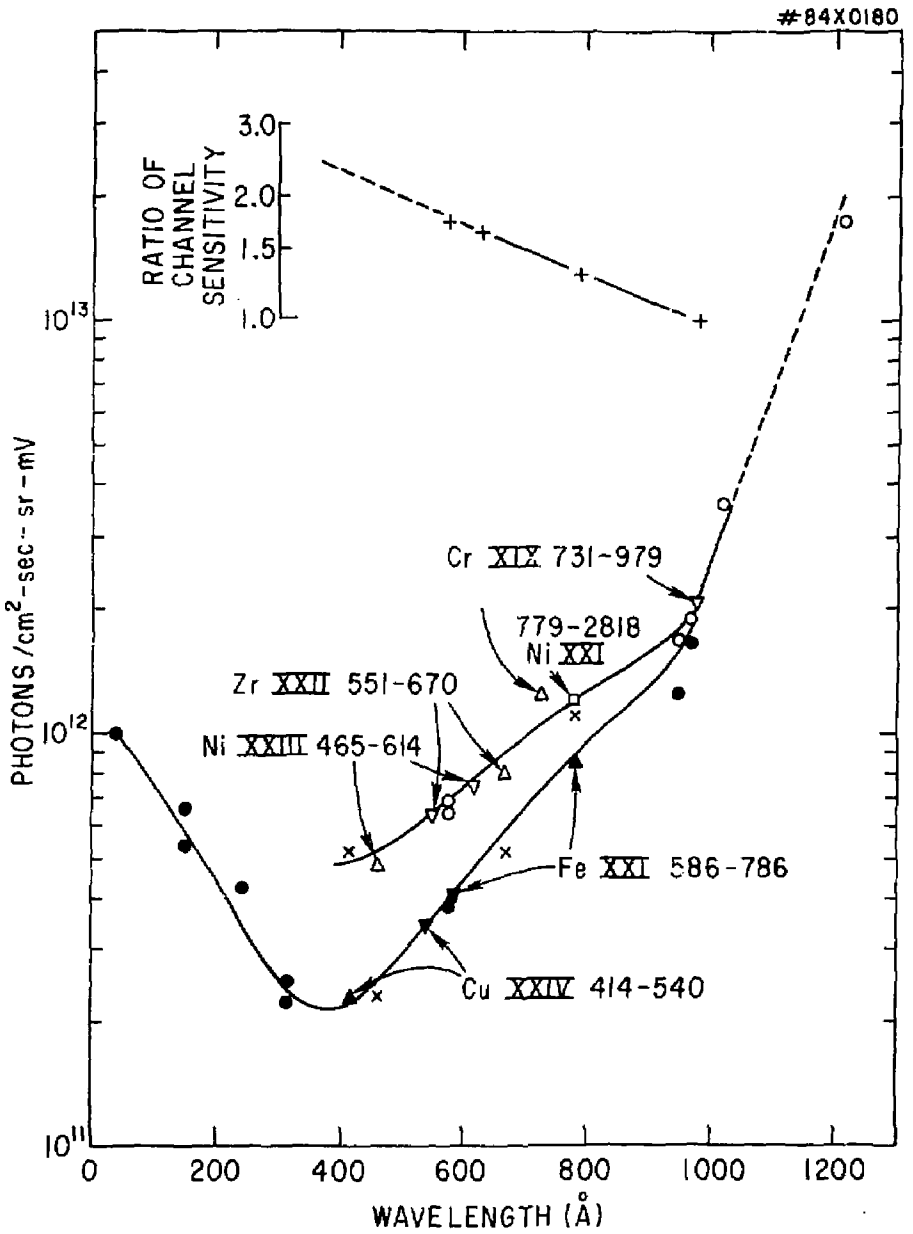
HI Lines

Fig. 1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10¹¹
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779-2818
Ni XXI
Zr XXII 551-670
Ni XXIII 465-614
Fe XXI 586-786
Cu XXIV 414-540
0
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400
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1000
1200
WAVELENGTH (Å)

Fig. 2

#84X0178

Cr XVIII

$2s^2 2p^3$ CONFIGURATION

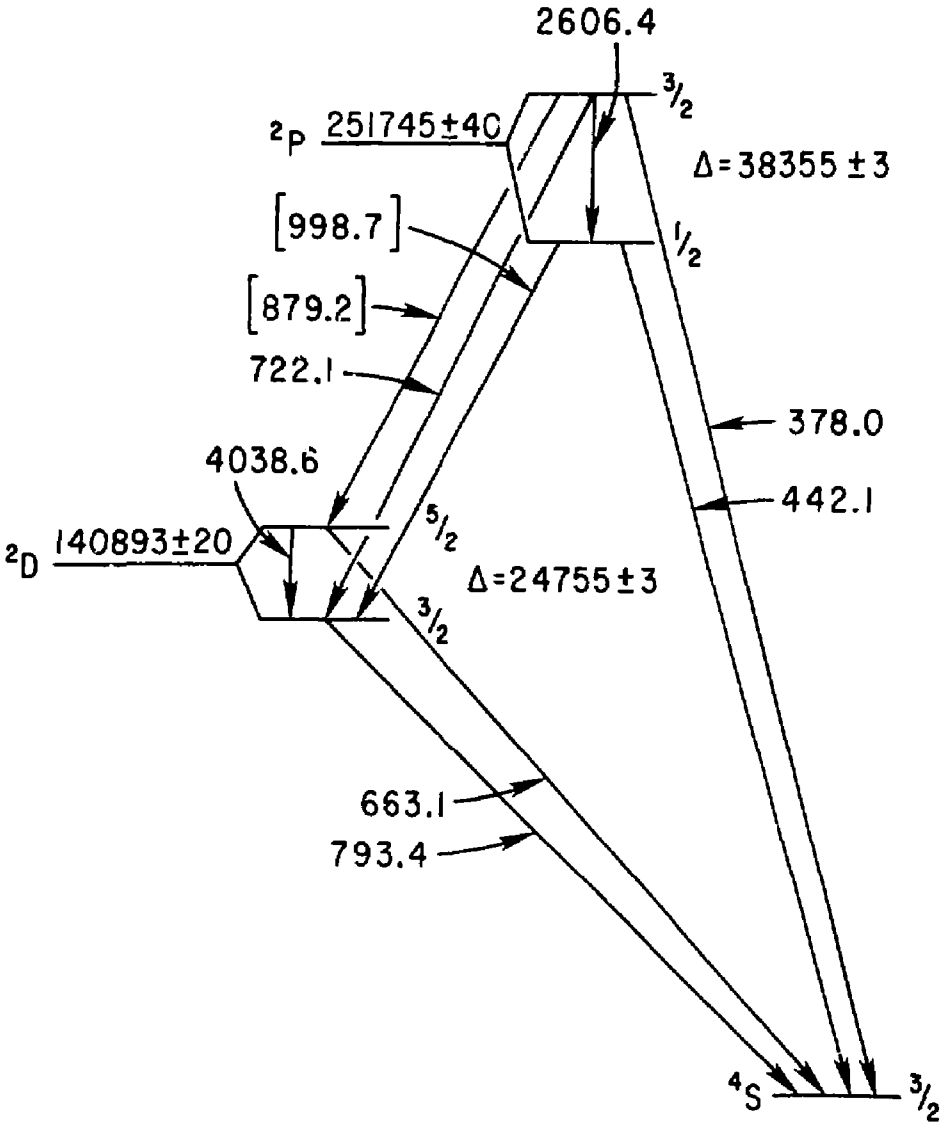

Fig. 3

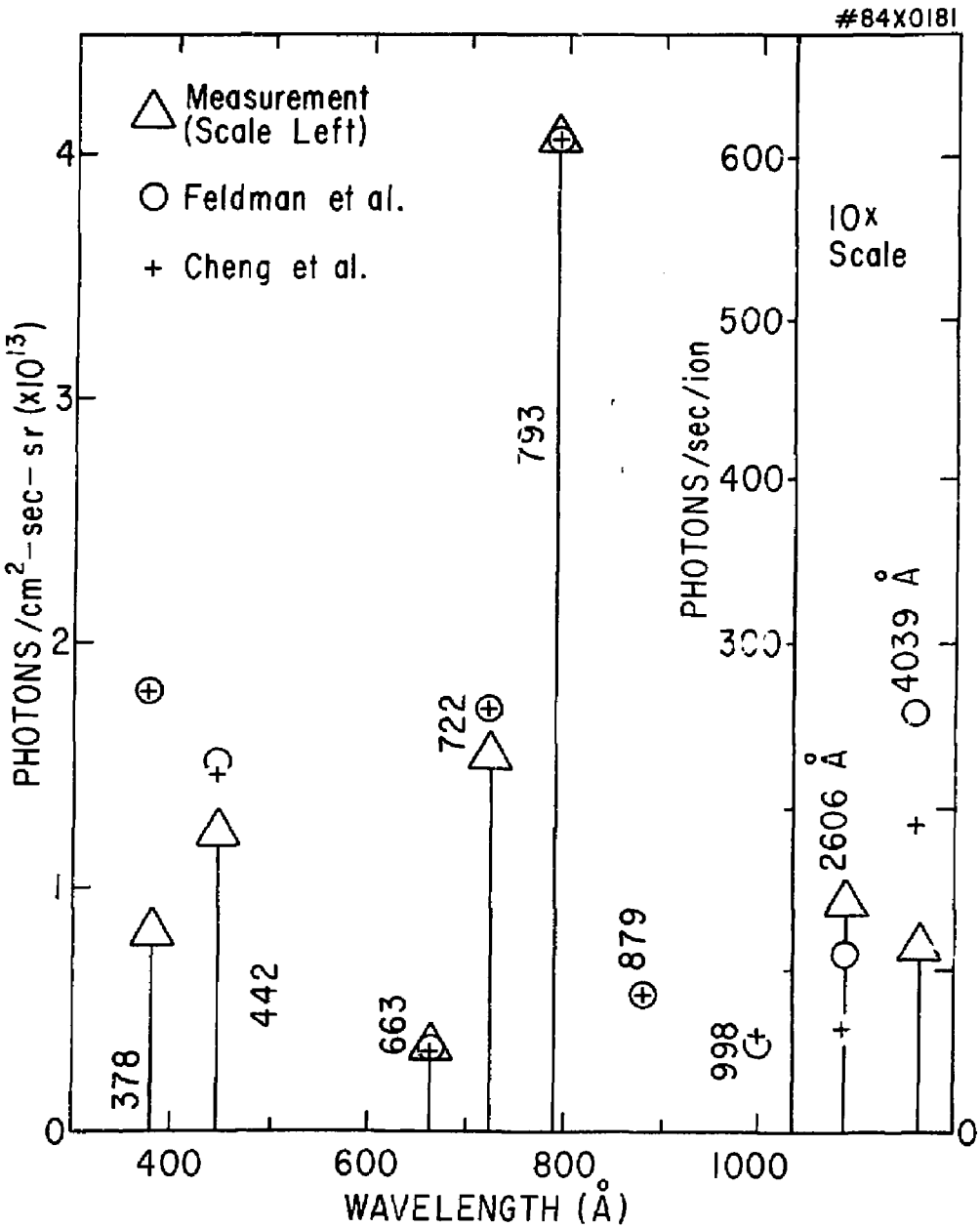
#84X0181
Measurement (Scale Left)
Feldman et al.
Cheng et al.
10x Scale
PHOTONS/cm²-sec-sr (x10¹³)
PHOTONS/sec/ion
WAVELENGTH (Å)
378
442
663
722
793
879
998
2606 Å
4039 Å
0
1
2
3
4
300
400
500
600
400
600
800
1000

Fig. 4

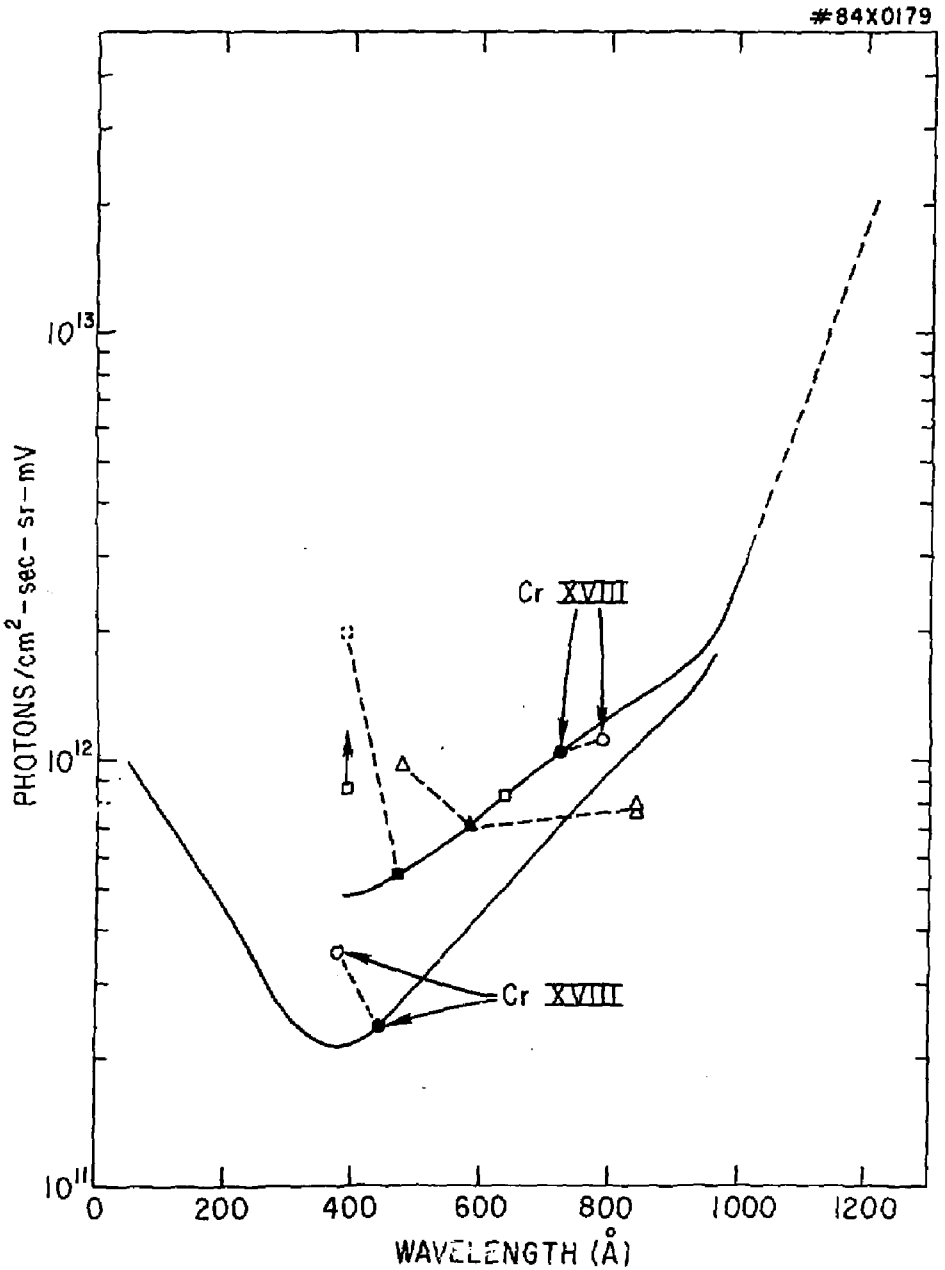
#84X0179
PHOTONS/cm²-sec-sr-mV
10¹³
10¹²
10¹¹
Cr XVIII
Cr XVIII
0
200
400
600
800
1000
1200
WAVELENGTH (Å)

Fig. 5

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