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New Classifications in Si-like Kr XXIII and Mo XXIX

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** See Appendix 1*

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ABSTRACT.

Radiation from Si-like Kr XXIII and Mo XXIX has been observed on the JET tokamak. In determining the ionization stages of the new transitions the temporal variation of the line intensities during discharges was investigated in detail. In the wavelength range 70–330Å, 11 new Kr XXIII and 11 new Mo XXIX lines were classified by means of isoelectronic analyses and comparisons with relativistic calculations. The results confirm and extend previous tokamak studies

1. Introduction

Recently, Sugar *et al.* [1] reported a comprehensive study of highly charged Si-like ions, in particular Cu XVI - Mo XXIX. The experimental data, from tokamak observations and laser-produced plasmas, were compared with theoretical *ab initio* calculations as well as with semiempirical data. Their work largely extended some previous tokamak-based studies of highly charged Si-like ions [2-4].

Several theoretical investigations of energies and oscillator strengths for Si-like ions have appeared in the literature. For instance, Biémont [5] and Fawcett [6] have applied the relativistic Hartree-Fock (HFR) code of Cowan [7] to these ions up to Ni XV. Their work was semiempirical in the sense that the Slater integrals were adjusted to optmize the agreement with experimental level energies. Using the multiconfiguration Dirac-Fock (MCDF) program of Desclaux [8], Huang [9] has performed fully relativistic *ab initio* calculations for Si-like ions in the range Z = 15 - 106.

In the present paper we report on new data for two spectra in the Si I sequence, namely Kr XXIII and Mo XXIX. The experiments were carried out at the JET tokamak. In analyzing the data, advantage was taken of previous experimental and theoretical work, in particular [1,9]. We also performed additional calculations, by applying the Cowan code to higher members of the sequence.

The structure of Si-like ions is quite interesting from the atomic physics point of view. There are 4 electrons outside the closed $2p^6$ shell and the number of configurations within the n = 3 complex is 12. The ground term is $3s^23p^2\ ^3P_{0,1,2}$, and there are two low-lying metastable levels, $3s^23p^2\ ^1D_2$ and $^1S_0$. Magnetic dipole (M1) transitions between these levels have been observed in the spectra of the solar corona and of tokamaks; for a critical compilation of such data see [10]. The lowest odd configurations are $3s3p^3$ and $3s^23p3d$, between which pronounced configuration interaction may occur. Previous work has shown that with increasing Z the $3s^23p^2$ - $3s3p^3$ transitions become relatively weak, the spectra being now dominated by the $3s^23p^2$ - $3s^23p3d$ lines [11]. This has been explained theoretically as quenching of a complete transition array by configuration interaction [12].

2. Experiment.

The experimental technique as well as the methods of data analysis have been described in a previous publication [13]. The plasma conditions were as follows: electron temperature T_e = 3-7 keV and electron density n_e = (3-6) x 10^{13} cm^{-3}. Of the ions studied here, Kr was deliberately introduced into the JET plasma, whereas Mo appeared accidentally in connection with neutral beam injection.

Spectra were recorded using a 2 meter grazing incidence spectrometer [14]. The spectral resolution (FWHM) was close to 0.25 Å, allowing wavelength determination with ±0.025 Å uncertainties in first grating order. Our line widths are thus larger than those obtained by Sugar *et al.* [1], but as a compensation for this, comparatively weak lines could be measured in the present experiment, including some new $3s^23p^2$ - $3s3p^3$ transitions.

In classifying the lines, the measured temporal variation of the line intensities during the discharge was found to be very useful in order to distinguish between different charge states. Figure 1 shows the temporal intensity variation for two Mo lines, one belonging to Mo XXIX and the other to Mo XXIV. In the case of Mo, accidental influxes of this element were generally sufficient enough to cause a large drop in the electron temperature (as seen in Fig. 1) and, indeed, would sometimes lead to a disruption of the plasma. In Fig. 1 the sudden decrease in electron temperature leads to a rearrangement of the ionization balance for Mo, which explains the "disappearance" of the Mo XXIX line around 11.5 s, and the concomitant increase in the intensity of the Mo XXIV line. As the temperature recovers, the higher ionization stages of Mo may be produced again; hence the increase in Mo XXIX intensity.

3. Results

A typical Kr spectrum is shown in Fig. 2. The transitions belonging to Mg-like Kr XXV and Al-like Kr XXIV have been discussed in our previous paper [13] in which additional spectra were shown. The new identifications in Kr XXIII and Mo XXIX are summarized in Table I. These classifications, (particularly in the case of Mo) are principally based on temporal intensity studies discussed above, comparisons with previous experimental data [1], the MCDF calculations [9] and our own calculations, using the Cowan program [7]. The difference between the experimental and theoretical excitation (or transition) energies is expected to vary smoothly with the net charge of the core ζ. In some cases it was necessary to extrapolate over several values of ζ, which may lead to substantial uncertainties. However, in doing this work we had access to some recent spectra of Si-like Sr XXV, recorded in high-temperature laser-produced plasmas [15], which provided support of our assignments. As pointed out earlier [13], the relative sensitivity of the detection system at different wavelengths has not been accurately determined. The intensity scale in Table I is therefore relatively crude, each of the intensity figures (1-4) covering an interval of the number of photons counted (for details see Table I).

Two examples of isoelectronic analyses are depicted in Figs. 3 and 4. For the transition shown in Fig. 3 previous data were available up to Kr. Our new point, for Mo, is supported by the Sr result [15]. A point to note in Fig. 3 is the deviation of the Fe measurement from the otherwise smooth curve, indicating a misidentification for this element. The situation illustrated in Fig. 4 is somewhat simpler, here Sugar *et al.* [1] provided data up to Zr and extrapolated these values to Nb and Mo, the latter now being confirmed. Several of the lines listed in Table I represent transitions between levels established in [1]; here the present data lend additional support to earlier assignments.

In the Kr XXIII spectrum, Sugar *et al.* [1] classified 11 lines as transitions between the $3s^23p^2$ - $3s^23p3d$ configurations and 1 line as the $3s^23p^2$ $^3P_2$- $3s3p^3$ $^3S^o_1$ combination. All these lines were observed in our spectra as well, along with the lines listed in Table I. The position of the $3s3p^3$ $^3S^o_1$ level is confirmed through our identification of the $3s^23p^2$ $^3P_{0,1}$ - $3s3p^3$ $^3S^o_1$ components, listed in Table I. For the $3s^23p^2$ $^3P_2$ - $3s^23p3d$ $^3P^o_2$ transition Sugar *et al.* [1] provide an interpolated value of 128.479 Å, in agreement with our measured wavelength 128.500 Å.

In the case of Mo XXIX, Sugar *et al.* [1] classified 5 lines, all of which appear in our spectra. There are additional Mo XXIX transitions for which extrapolated wavelengths are given in [1]. Our experimental values are in reasonable agreement with these predictions. A number of additional lines are listed in Table I. However, as will be discussed below, some of the assignments are tentative, because of the lack of observations for adjacent ions.

The excitation energies of the newly established levels are given in Table II. These data are in satisfactory agreement with the results of MCDF calculations [9].

4. Discussion

4.1. The $3s3p^3$ levels. Of the 6 possible terms of this configuration only $3s3p^3\ ^3S^o_1$ has been observed for spectra beyond As XX [1]. As noted above, we have observed additional decays of this level in Kr XXIII and Mo XXIX.

The $3s3p^3\ ^5S^o_2$ level which is the lowest of all the $3s3p^3$ levels has only one radiative decay mode, namely through spin-forbidden E1 transitions to $3s^23p^2\ ^3P_{1,2}$. For several years efforts were made [16] to locate these lines for spectra beyond S III, but only recently were conclusive experimental data obtained, for a number of ions from Ar V to Zn XVII, by means of time-delayed beam-foil spectroscopy [17]. Besides being observable in such experiments, the intercombination lines in Fe XIII also appear in the spectra of solar flares [18,19]. We have now observed these lines in the tokamak spectra of Kr XXIII and Mo XXIX. In the Kr case the two lines, at 250.08 and 267.51 Å have the theoretically expected intensity ratio [9] and their wavenumber difference corresponds to the known $3s^23p^2\ ^3P_{1,2}$ fine structure. In Mo only one of the two lines, at 185.65 Å, was observed, the other one falling outside the wavelength range studied. However, the somewhat tentative assignment is supported by the temporal variation of the line intensity and the fact that there were no other unidentified lines in the region of interest. It should be added that similar intersystem lines, in Al-like ions, were observed in our previous study [13].

Figure 5 shows an isoeletronic plot of the difference between the measured and calculated [9] excitation energies of the $3s3p^3\ {}^5S^o_2$ term. It has been noted earlier [17] that this difference is about 3 800 cm^{-1}, practically independent of Z. However, Fig. 5 shows that it tends to decrease linearly for ions beyond Ni XV. This is not surprising because the accuracy of the MCDF calculations is expected to improve as Z increases. We have performed an isoelectronic smoothing of the ${}^3P_{1,2} - {}^5S^o_2$ transitions, by fitting the differences Δ between experimental and theoretical [9] wavenumbers to polynomials of ζ (the net charge of the core). For instance, the relation $\Delta = 2930 + 251.2\zeta - 18.5\zeta^2 + 0.28\zeta^3$ was obtained for the ${}^3P_1 - {}^5S^o_2$ transition. In Table III the measured and fitted wavelengths are given for the spectra Ti IX - Mo XXIX. Some years ago, Hinnov [20] provided tentative wavelengths of these transitions in Si-like Fe, Ge, Se and Mo. With the possible exception of Fe, those early data are in quite satisfactory agreement with the present results. It is also worth noting that the wavenumber differences of the fitted transitions are in very good accord with the ${}^3P_1 - {}^3P_2$ fine-structure separations, as determined from tokamak observations of M1 transitions [1,21-23]. The data in Table III ought therefore to be valuable in future studies of intercombination lines in Si-like ions.

We have further assigned some lines to transitions from additional $3s3p^3$ levels, viz. ${}^3P^o_2$ and ${}^1D^o_2$, see Tables I and II. These identifications involve a substantial isoelectronic extrapolation and must be regarded as tentative, however.

4.2. The $3s^23p3d$ levels. The levels of this configuration are $^1P^o_1$, $^3P^o_{1,2,3}$, $^1D^o_2$, $^3D^o_{1,2,3}$, $^1F^o_3$ and $^3F^o_{2,3,4}$. Here significant mixing occurs, in particular for levels with J = 1 ($^3P^o_1$ and $^3D^o_1$) and J = 2 ($^3D^o_2$ and $^1D^o_2$), see [1].

We have now obtained data for the $3s^23p3d$ $^1P^o_1$ level in Kr XXIII and Mo XXIX. In both ions transitions to $3s^23p^2$ $^1S_0$ were identified. The results are corroborated by observations of laser-produced plasma spectra for Sr XXV [15].

The $3s^23p3d$ $^3P^o_1$ level energy in Mo XXIX is determined from a single line. However, the difference between the experimental and theoretical energies (in Huang's paper [9] the level is labeled as $^3D^o_1$) varies smoothly with Z, supporting the assignment. A search for the $3s^23p3d$ $^3D^o_1$ level (which is known up to Kr XXIII [1]), did not provide conclusive results for Mo XXIX, largely because of blending from lines belonging to lower ionization stages in the JET spectra. The same reason precludes a determination of the energy of the $3s^23p3d$ $^3D^o_2$ level in Mo XXIX for which an extrapolated value is available [1]. For three other levels of this confguration, $^1D^o_2$, $^3D^o_3$ and $^1F^o_3$, which were experimentally established in Mo XXIX [1], some additional decay channels were observed in the present work.

4.3. Forbidden lines. Sugar *et al.* [1] provide a comprehensive, critically evaluated list of M1 transitions in Si-like ions. This material extends and updates previous such data [10]. The $3s^23p^2(^3P_1$ - $^1S_0)$ M1 transition in Mo XXIX is of particular interest in the present case. A tokamak observation [21] here yielded a tentative wavelength of 325.3 Å, whereas Sugar *et al.* [1] propose 326.3 ± 0.3 Å. The latter value is based on isolectronic analyses. We studied the JET spectra carefully, but it is not yet possible to provide a definite answer. We have observed a line at at 325.22 Å, in excellent agreement with [21], but due to the observation conditions (disrupting plasma) the spectrum also contains Mo lines from comparatively low charge states, and there is a strong Mo XI transition at exactly this wavelength [24]. It is unsatisfactory that the energy of the important $3s^2 3p^2\ ^1S_0$ term is not on a firmer experimental basis, and we are therefore continuing the search for it.

5. Concluding remarks.

In addition to the transitions in Si-like Kr and Mo classified in this study we have found several other lines in the spectra from JET which most likely are transitions in these ions. However, definite classifications are at present precluded because of lack of data for lower ionization stages. As an example, the $3s^2 3p3d\ ^3F^o_{2,3,4}$ levels deserve mentioning. Of these $^3F^o_4$ is metastable, whereas $^3F^o_2$ and $^3F^o_3$ decay to the $3s^2 3p^2\ ^3P_{1,2}$ levels. In a beam-foil lifetime study of Ni XV [25] such transitions were tentatively identified but for no other spectrum do similar data exist. We have candidates for these decays in Mo XXIX but more work is needed before definite conclusions can be drawn. This is in an interesting contrast to the $3s^2 3p3d\ ^1F^o_3$ case; as noted transitions from this level have been observed for several spectra up to Mo XXIX. In summary, the present results have extended the comprehensive work of Sugar *et al.* [1] and both investigations confirm again that tokamaks are highly competitive light sources for accurate spectroscopy of highly charged ions. It would now be interesting to extend the work to charge states higher than Mo XXIX. Only for Ag XXXIV, where some M1 lines were observed [23], is experimental material available at present.

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Table I. *New identifications in Kr XXIII and Mo XXIX*

Spectrum	Intensity[a]	Wavelength (Å)	Identification
Kr XXIII	1	111.051	$3s^23p^2\ ^3P_1$ - $3s^23p3d\ ^3D^o_2$
	3	114.39	$^3P_2$ - $^3D^o_2$
	3	124.52	$^1S_0$ - $^1P^o_1$
	1	127.288	$^3P_0$ - $3s3p^3\ ^3S^o_1$
	2	128.500	$^3P_2$ - $3s^23p3d\ ^3P^o_2$
	1	132.789	$^1D_2$ - $^1D^o_2$
	3	139.42	$^3P_1$ - $3s3p^3\ ^3S^o_1$
	1	170.85[b]	$^3P_2$ - $^3P^o_2$
	2	179.30[b]	$^1D_2$ - $^1D^o_2$
	1	250.08	$^3P_1$ - $^5S^o_2$
	2	267.51	$^3P_2$ - $^5S^o_2$
Mo XXIX	2	80.922	$3s^23p^2\ ^3P_2$ - $3s^23p3d\ ^1F^o_3$
	3	82.951	$^3P_1$ - $^3P^o_1$
	3	86.014	$^3P_1$ - $^3P^o_0$
	3bl	89.52	$^3P_0$ - $3s3p^3\ ^3S^o_1$
	2	98.458	$^1S_0$ - $3s^23p3d\ ^1P^o_1$
	3	100.703	$^3P_2$ - $^3P^o_2$
	2	104.704	$^3P_1$ - $3s3p^3\ ^3S^o_1$
	2	105.780	$^1D_2$ - $3s^23p3d\ ^3D^o_3$
	3	127.57[b]	$^3P_2$ - $3s3p^3\ ^3P^o_2$

Table I (cont).

4	141.20[b]	$^1D_2$ -	$^1D^o_2$
2	185.65	$^3P_1$ -	$^5S^o_2$

[a]The intensity figures 1-4 are related to the number of counts (above background) at the peak positions of the lines as follows:
1 = 20-50 counts, 2 = 60-200 counts, 3 = 210-600 counts and 4 = 610-3000 counts. A blended line is denoted by bl.

[b]Tentative assignment (see text).

Table II. *Energies (cm^{-1}) in Si-like Kr XXIII and Mo XXIX.*

Level		Kr XXIII	Mo XXIX
$3s3p^3$	$^5S^o_2$	468 240	700 370
	$^3P^o_2$	679 710	980 800
	$^1D^o_2$	743 210	1 093 700
$3s^23p3d$	$^3P^o_2$		1 189 990
	$^3P^o_0$		1 329 400
	$^3P^o_1$		1 367 250
	$^1P^o_1$	1 057 580	1 483 880

Table III. *Observed and fitted wavelengths (Å) of the* $3s^2 3p^2\ ^3P_{1,2}$ - $3s3p^3\ ^5S^o_2$ *intercombination transitions in Ti IX - Mo XXIX.*

Ion	$^3P_1 - {}^5S^o_2$		$^3P_2 - {}^5S^o_2$	
	λ (obs)	λ (fit)	λ (obs)	λ (fit)
Ti IX	703.68 (50)	703.00	724.42 (25)	724.29
V X		635.40		657.32
Cr XI	578.8 (8)	578.35	600.7 (4)	600.78
Mn XII	529.79 (5)	529.46	552.84 (40)	552.25
Fe XIII	487.08 (3)	487.08	510.4 (3)	510.07
Co XIV	450.14 (10)	449.97	472.99 (7)	472.98
Ni XV	416.92 (10)	417.18	439.86 (10)	440.04
Cu XVI	387.56 (40)	388.03	410.46 (40)	410.58
Zn XVII	361.96 (40)	361.96	383.77 (30)	383.99
Ga XVIII		338.42		359.90
Ge XIX		317.20		337.97
As XX		297.97		317.95
Se XXI		280.49		299.63
Br XXII		264.57		282.86
Kr XXIII	250.08 (3)	250.06	267.51 (3)	267.49
Rb XXIV		236.81		253.40
Sr XXV		224.78		240.58
Y XXVI		213.62		228.64
Zr XXVII		203.48		217.77
Nb XXVIII		194.18		207.80
Mo XXIX	185.65 (3)	185.65	198.63 (3)[a]	198.64

[a]Computed value, using the 185.65 Å line and known $^3P_2 - {}^3P_1$ separation.

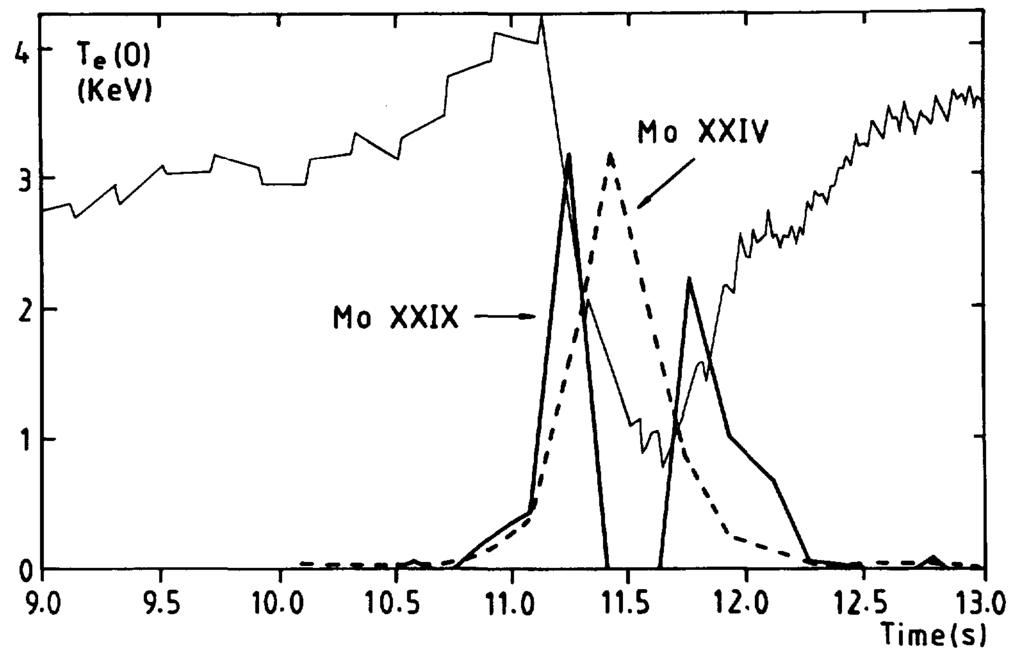

Fig. 1. Temporal intensity variation of a Mo XXIV and a Mo XXIX line during a discharge. At t = 10.5 s neutral beam injection, P_{NBI} = 4 MW, was initiated. The central electron temperature is indicated. The intensity scale for the two Mo transitions is linear but the peak intensities have been normalized to the same value.

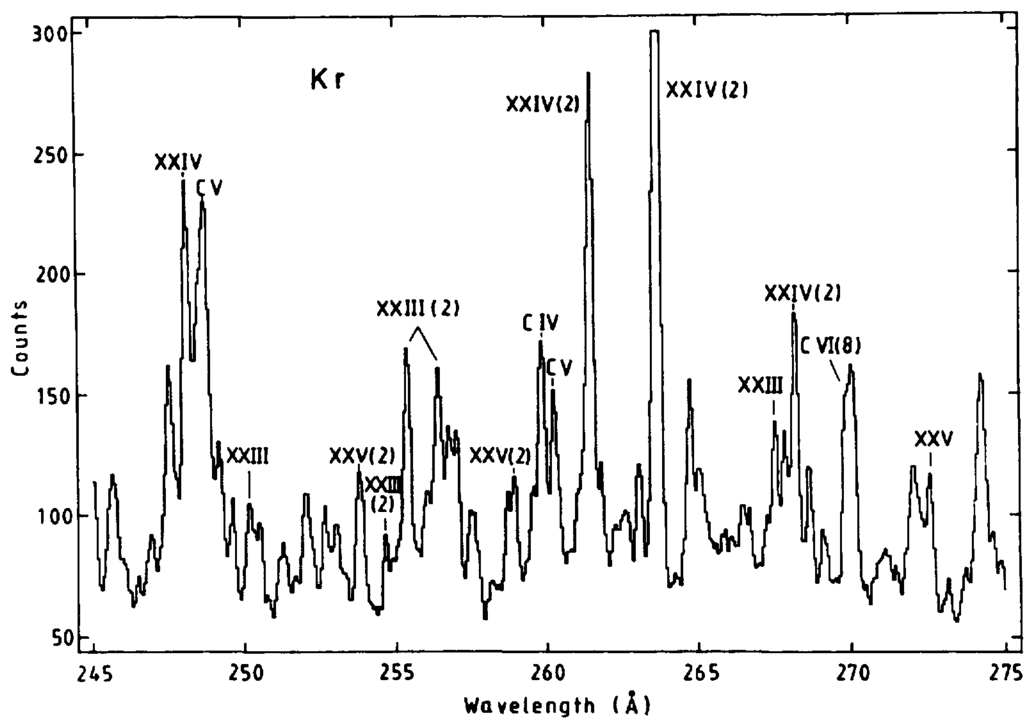

Fig. 2. Partial spectrum, dominated by Kr transitions. The spectrum numbers and diffraction orders of the lines are indicated.

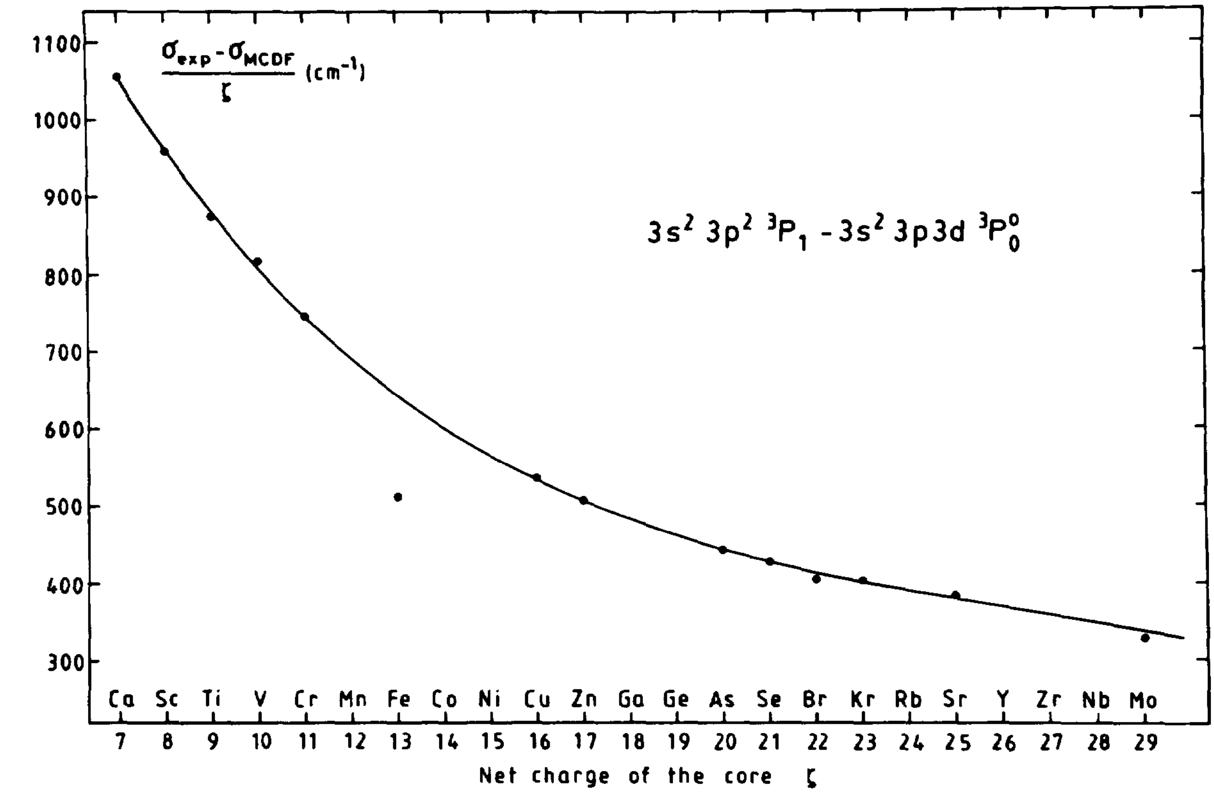

Fig. 3. Isoelectronic plot of the $3s^23p^2\;{}^3P_1$ - $3s^23p3d\;{}^3P^o_0$ transition in Si-like ions.

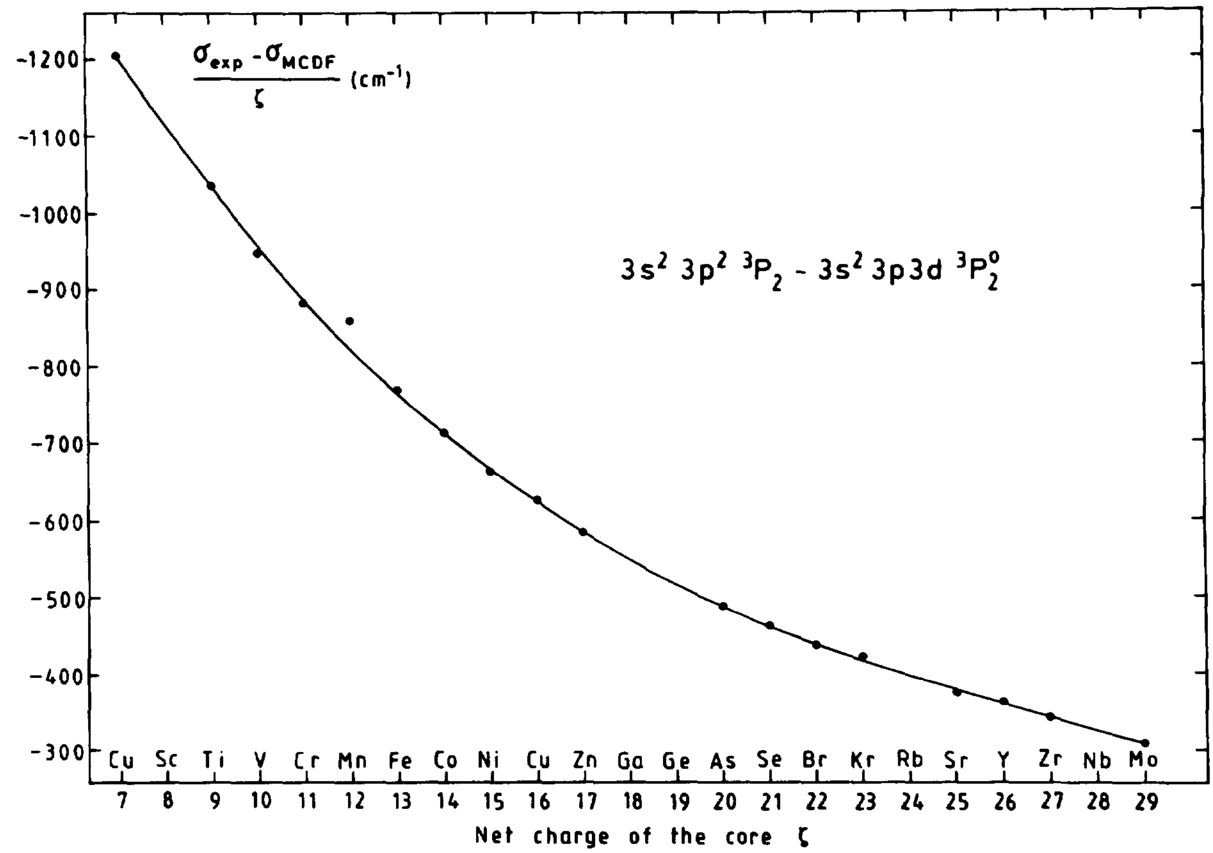

Fig. 4. Isolectronic plot of the $3s^23p^2\;{}^3P_2$ - $3s^23p3d\;{}^3P^o_2$ transition in Si-like ions.

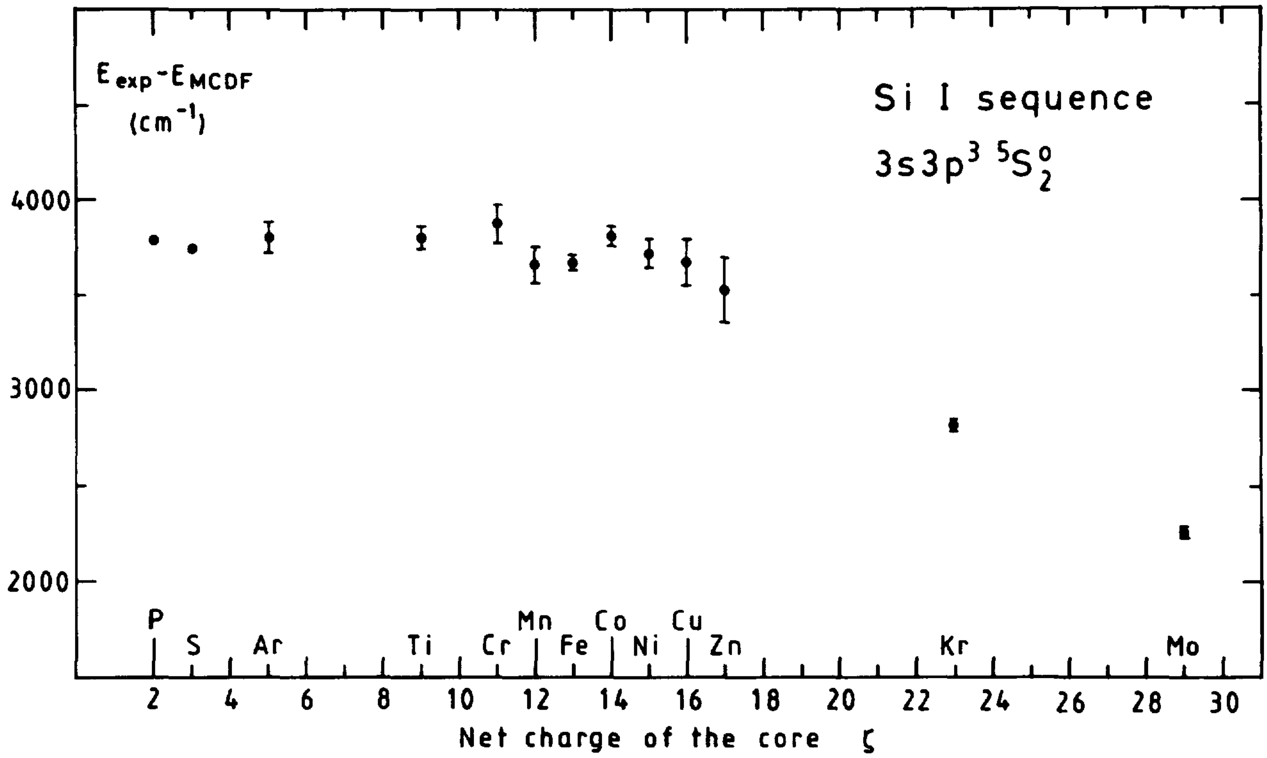

Fig. 5. Difference between experimental and theoretical excitation energies of the $3s3p^3\ {}^5S^o_2$ level in Si-like ions.

APPENDIX 1.

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