THE STRANGE AND EMOTIONAL STORY OF Mo VI – UNUSUAL CONTRIBUTIONS TO THE SPECTRUM ANALYSIS FOR RUSSIA, SWEDEN, AND THE U.S.A.

Joseph Reader

National Institute of Standards and Technology, Gaithersburg, Maryland

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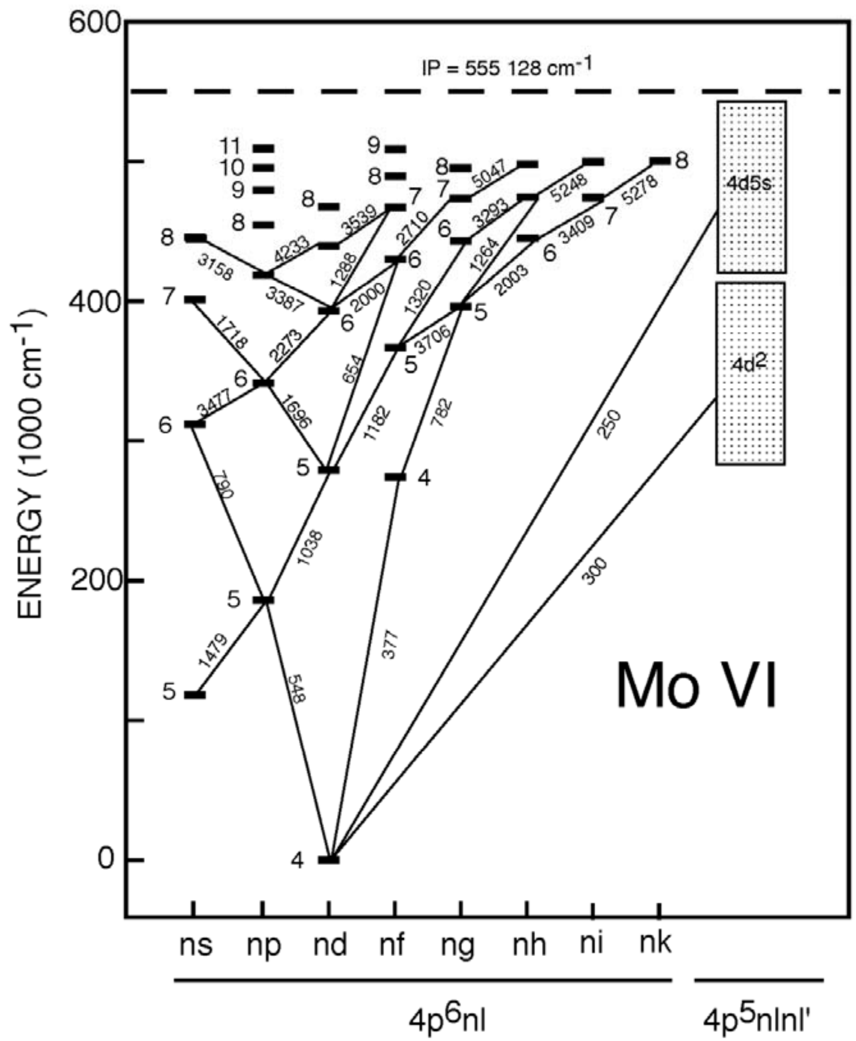

Mo VI
IP = 555 128 cm-1
ENERGY (1000 cm-1)
0
200
400
600
ns
np
nd
nf
ng
nh
ni
nk
4p6nl
4p5nlnl'
4d5s
4d2

HISTORY OF Mo VI

TRAWICK (1934); spark	4d, 5s, 5p, 5d, 6s
CHARLES (1950); spark	4f
ROMANOV & STRIGANOV (1969) Penning discharge	6p, 7p, 6d, 7d, unconnected hydrogenic
MUSTAQ et al. (1979); spark	$4p^64d$-$4p^54d5s$
TAUHEED et al. (1985); spark	$4p^64d$-$4p^54d^2$; long wavelengths CI
EDLÉN et al (1985).; spark	7s, 5f, 5g, 6g, connected hydrogenics (6h, 7h, 7i, 8i, 9i, 8k, 9k)
KANCEREVICIUS et al. (1991); semi-sliding spark	8p, 9p, 10p, 11p, 6f, 7f, 8f, 9f, 10f, $4p^54d^2$, $4p^54d5s$

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14 May 1985

Dear Joe,

You may be interested in this paper, especially in the discovery of an unexpected perturbation of the ng ^2G series, which has consequences for the series limit determinations in other members of the isoelectronic sequence. The paper will appear in Physica Scripta.

Best regards to you and the family.

Yours
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Bengt Edlén (1906-1993) with King Gustav VI Adolf

Physica Scripta. Vol. 32, 215–219, 1985

Extended Analysis of Mo VI

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Abstract

The analysis of the RbI-like spectrum Mo VI has been extended to include a total of some 110 classified lines and 44 energy levels belonging to the one-electron configurations $4s^2 4p^6(^1S)nl$ with n ranging up to 9 and l up to 7. The analysis is based on recordings of vacuum spark spectra made at Lund in the region 230–2350 Å, complemented by a list of lines from 2193 to 6336 Å observed and identified by Romanov and Striganov in a Penning type arc discharge. The one-electron level system is partly mixed with core-excited configurations, not treated in the present paper. Especially the nf series is strongly perturbed by $4s^2 4p^5 4d^2$, and an anomalous behaviour of the ng series is explained by interaction with the ^2G term of $4s4p^6 4d^2$. The ionization limit, derived from $6h$, $7i$ and $8k$ by means of the polarization formula, is found to be $555\,132 \pm 2\,\mathrm{cm}^{-1}$.

1. Introduction

The sixth spectrum of molybdenum, Mo VI, is isoelectronic with RbI and consists in the first place of the one-electron configurations $4s^2 4p^6(^1S)nl$ with $4d\,^2D$ as ground term. However, core-excited configurations, especially $4s^2 4p^5 4d^2$, are also responsible for an important part of the spectrum. The present paper deals only with the one-electron system, while the configuration $4s^2 4p^5 4d^2$ is treated in ref. [11].

The early work by Trawick [1] and Charles [2] had led to the identification of 13 lines in the region 374–1595 Å, connecting the ten lowest levels of the system. An important addition to the knowledge of Mo VI was provided by Romanov and Striganov [3] by observing a number of lines in the long-wave region emitted by a Penning type arc discharge. Besides adding 6, 7p and 6, 7d to the term system they observed a large part of the "hydrogenic tail" of the spectrum, including ng, nh, ni and nk orbits, evidently favoured by their light source. However, the observed transitions were insufficient to interconnect the different pairs of levels involved and to connect them to the rest of the term system. As a result of the pesent investigation these connections have now been established, which has made it possible to derive an accurate value for the series limit.

2. Experimental details

Our line list is mainly based on recordings made with a 3-m normal incidence spectrograph at Lund. We used an aluminium-coated grating for the region 400–2540 Å and a goldcoated grating, with higher reflectance for the shorter wavelengths, for 250–1650 Å. Both gratings have 1200 lines/mm, giving a plate factor of 2.8 Å/mm. Open and sliding vacuum sparks were operated with a 0.5 μF condenser at about 40 and 8–15 kV respectively.

The reported line intensity figures are from visual estimates of the photographic blackening, uncorrected for the λ-dependence of recording efficiency. The ion affiliation of the observed lines is found from a study of the intensity variation of the lines caused by additional inductance introduced in the discharge circuit in steps of 4, 10 and 15 turns of an induction coil. The intensity of Mo VI lines shows little variation, while the Mo VII lines decline considerably at 15 turns (about 0.1 mH) and those of Mo V get enhanced.

3. The analysis

The analysis started with a verification of the previously established levels, including those of 6, 7p and 6, 7d found in ref. [3]. After a preliminary derivation of the series limit, about $6000\,\mathrm{cm}^{-1}$ higher than the previously assumed value, the terms $ng\,^2G$ could be predicted with sufficient accuracy to permit

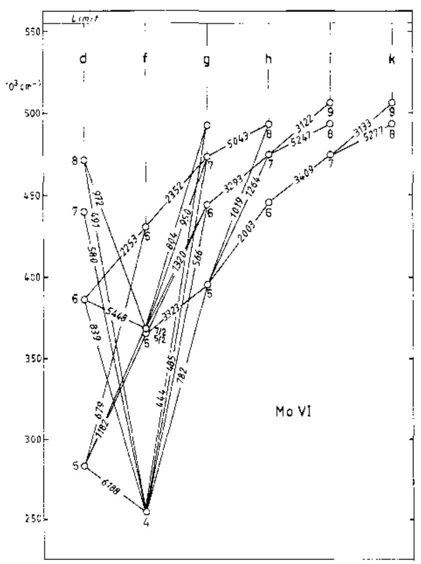


Fig. 1. Partial term diagram of the one-electron system of Mo VI.

Taj Mahal, India, 2005

K. Rahimullah, Adil Ahmad, Sabra Khatoon, S. M. Afzal, M. S. Z. Chaghtai

K. Rahimullah, Adil Ahmad, Evelyn and Joe Reader, Sabra Khatoon, M. S. Z. Chaghtai, Tauheed Ahmad

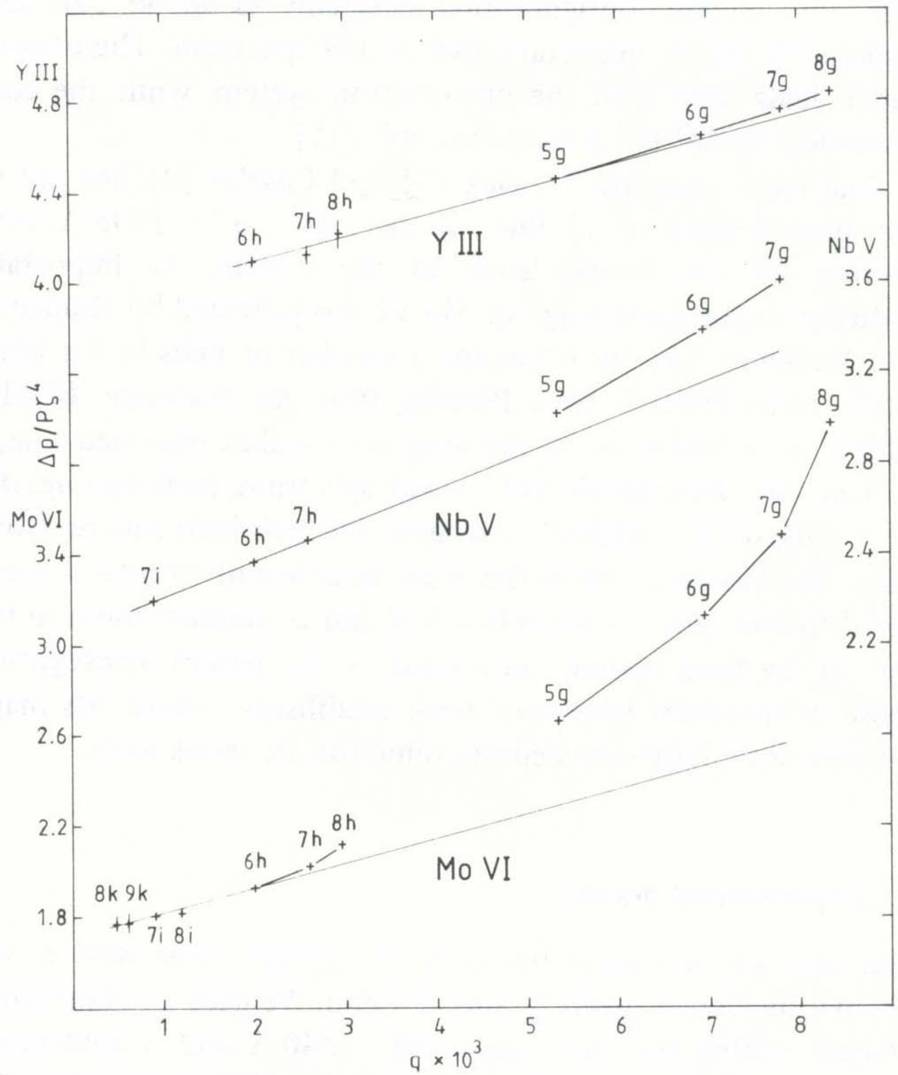


Fig. 4. Comparison of polarization diagrams for YIII, Nb V and Mo VI, normalized by the factor ζ^{-4} ($\zeta = Z - 36$). The anomalous behaviour of the ng series is explained by interaction with the ^2G term of $4s4p^6 4d^2$.

"The anomalous behaviour of the ng series is explained by interaction with the ^{2}G term of $4s4d^6 4d^2$."

2/26/93

Opt. Spectrosc. 27, 8-11 (1969)

JM

UDC 535.33 : 546.77.1

SPECTRUM OF Mo VI IN THE 6800–2200 Å REGION

N. P. Romanov and A. R. Striganov (pp. 17–24)

Received 6 November 1968

The molybdenum spectrum was excited in a Penning type arc discharge. The separation of lines according to ionization stages was carried out using the distribution of line emission along the discharge. In the 6800–2200 Å region, the wavelengths and relative intensities for 42 lines of Mo VI (Rb I isoelectronic sequence) were measured and 23 of them were classified. Four new energy levels of the Mo^{5+} ion were determined and values of previously known levels were refined.

In Ref. 1, an arc source of multiply charged ions (OIYaI) was investigated by methods of optical spectroscopy. It was observed that with an increase in voltage of the arc, the lines of tungsten and molybdenum appear in the discharge spectrum observed through the emission slit in the wall of the chamber, along with the lines of the working gas. These elements enter into the discharge as a result of the sputtering of the cathode and anticathode. In this case, the presence of tungsten and molybdenum ions is also established in the center of the discharge with the aid of mass-spectral analysis. An analysis of the distribution of these ions according to ionization stages showed that the W^{6+} ions give the highest current as compared to currents of ions in other ionization stages.[2] For molybdenum, the maximum current is obtained for Mo^{4+} ions.

Spectra of multiply charged molybdenum ions were studied only in the vacuum ultraviolet[3–6] where they were excited by a condensed vacuum spark. Therefore, it is of great interest to investigate the spectra of molybdenum ions in the visible and ultraviolet regions using a source of multiply charged ions.

DESCRIPTION OF EXPERIMENT

In the present work, the spectrum of molybdenum was investigated in the 6800–2200 Å region. The spectrum was excited in an arc discharge with a heated cathode and with electrons oscillating in a magnetic field[1] at an arc current of 5 A and a voltage of 400 V. Helium was used as the working gas. Its spectrum has few lines, thereby decreasing the probability of covering the molybdenum lines with gas lines. The spectrum was recorded on SP-II plates and on an "izopanchrom" photofilm using a DFS-8 spectrograph with a 1200 groove/mm diffraction grating (dispersion—3 Å/mm). The region of investigation was limited at the short wavelength end by the absorption of light in the spectrograph, and at the long wavelength end by the sensitivity of the photographic materials. For studying the line intensity distribution along the discharge, the image of the arc column was projected by a spherical mirror on the slit of the spectrograph. For exposures of the distribution across the discharge, the image was rotated 90° by a system of mirrors.

SEPARATION OF LINES OF IONS IN VARIOUS STAGES OF IONIZATION

Figure 1 gives a portion of the discharge spectrum close to the anticathode. Figure 1, a shows the line intensity distribution along the discharge, and Fig. 1, b shows the distribution across the discharge. In both cases, the change in line intensities essentially depends on the ion to which the line belongs. From the spectrogram in Fig. 1, a it is seen that the discharge spectrum around the anticathode is mainly composed of molybdenum lines, where the line intensities of Mo I and Mo II rapidly

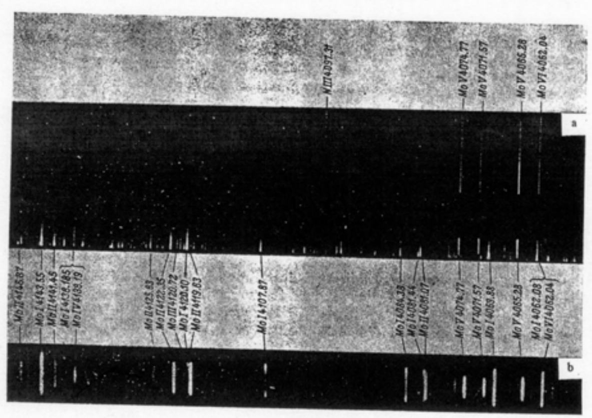


Fig. 1. Intensity distribution of spectral lines in the 4140–4060 A region. a—Spectrum along the arc column (at the bottom—anticathode, discontinuity along the length of the spectrum is caused by the shielding of the column); b—spectrum across the discharge at distance 4 mm from the anticathode.

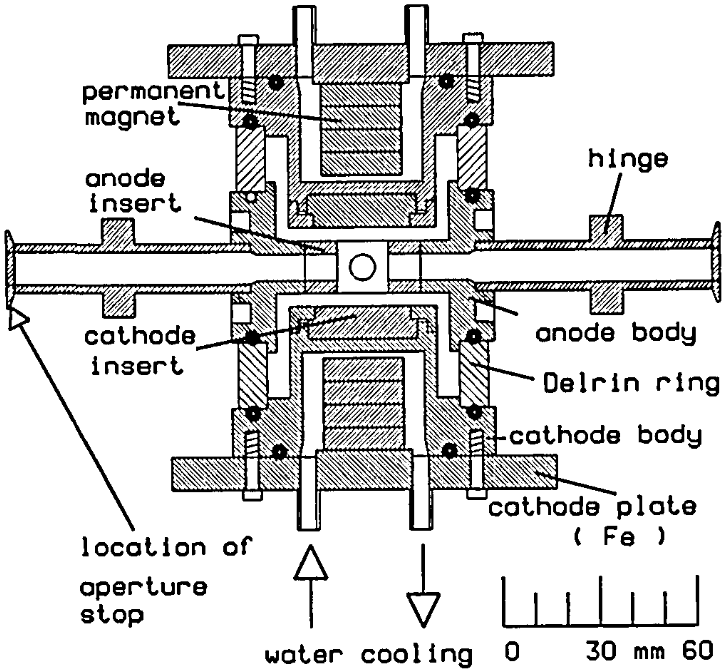


Fig. 1. Sectional drawing of the double-cathode Penning source. The two permanent magnets behind the cathodes attract each other so that the magnetic field is parallel to the electric field of the cathode falls. The anode body has four view ports at right angles for pumping, gas inlet, and observation.

HEISE et al. APPLIED OPTICS (1994)

E. Kononov, A. Striganov, L. Ivanov, E. Ivanova
Spectroscopy Council offices (1983)

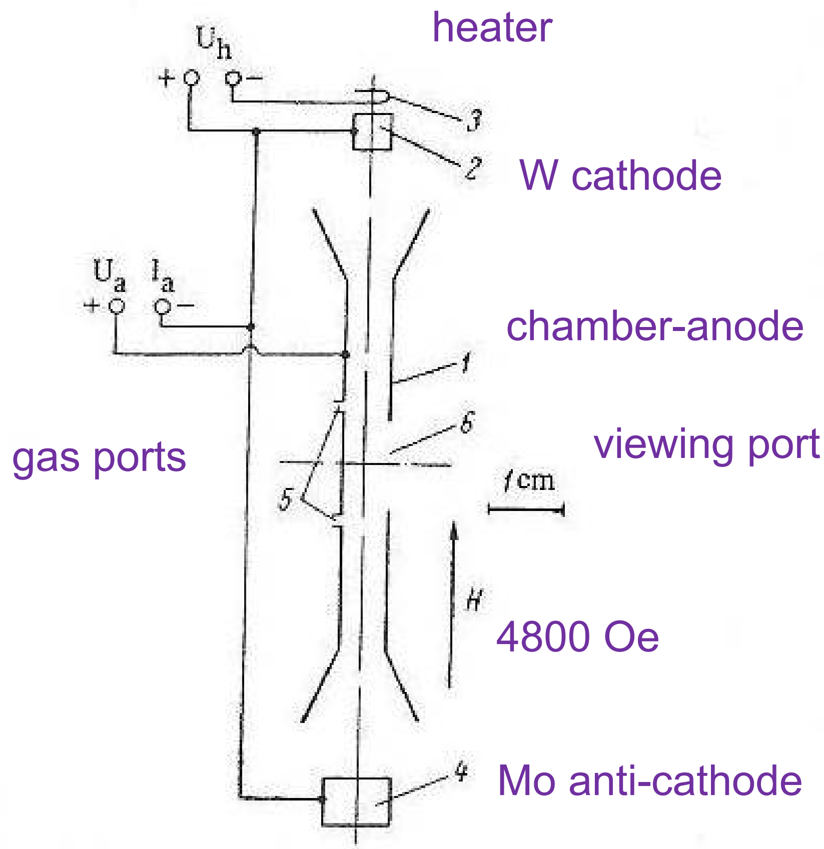


Fig. 1. Diagram of the multiply charged ion source.

Romanov and Pasyuk (1968)

Table 1. Mo VI Lines in the 6800–2200 Å Region

λ_{air} Å	Intensity	ν_{vac}, cm^{-1}	Transition
6336.04	5	15778.36	$4f\,^2F^\circ_{5/2}$—$5d\,^2D_{3/2}$
6328.11	1.5	15798.14	
6198.21*	1.4	16129.23	
6195.84*	1.8	16135.39	
6189.16*	1.8	16152.80	
6188.67	11	16154.10	$4f\,^2F^\circ_{7/2}$—$5d\,^2D_{5/2}$
6166.09*	1.6	16213.25	
6035.62	0.75	16563.72	$4f\,^2F^\circ_{5/2}$—$5d\,^2D_{5/2}$
5871.37*	1.5	17027.08	
5619.63*	1.7	17789.82	
5585.08*	1.0	17899.87	
5448.82	7.5	18347.51	
5355.81	2.5	18666.11	
5276.86*	45	18945.40	$7i\,^2I_{13/2,\,15/2}$—$8k\,^2K^\circ_{15/2,\,17/2}$
5247.45*	35	19051.57	$7h\,^2H^\circ_{11/2,\,13/2}$—$8i\,^2I_{13/2,\,15/2}$
5043.55*	10	19821.77	$7g\,^2G_{11/2}$—$8h\,^2H^\circ_{11/2,\,13/2}$
5042.77*	8.5	19824.84	$7g\,^2G_{9/2}$—$8h\,^2H^\circ_{11/2}$
4501.73*	1	22207.45	
4495.55*	9	22237.98	
4490.73*	11	22261.83	
4272.95	8	23396.45	$7p\,^2P^\circ_{3/2}$—$7d\,^2D_{3/2}$
4232.04	100	23622.63	$7p\,^2P^\circ_{3/2}$—$7d\,^2D_{5/2}$
4062.04	60	24611.24	$7p\,^2P^\circ_{1/2}$—$7d\,^2D_{3/2}$
4054.55	3	24656.68	
3735.32	90	26763.85	$6s\,^2S_{1/2}$—$6p\,^2P^\circ_{1/2}$
3538.39	20	28253.37	
3510.27	6.6	28479.68	
3484.77	13	28688.10	$6d\,^2D_{3/2}$—$7p\,^2P^\circ_{1/2}$
3476.60	200	28755.50	$6s\,^2S_{1/2}$—$6p\,^2P^\circ_{3/2}$
3411.11	25	29307.59	
3408.60*	200	29329.11	$6h\,^2H^\circ_{11/2,\,13/2}$—$7i\,^2I_{13/2,\,15/2}$
3386.98	20	29516.39	$6d\,^2D_{5/2}$—$7p\,^2P^\circ_{3/2}$
3343.20	1.5	29902.89	$6d\,^2D_{3/2}$—$7p\,^2P^\circ_{3/2}$
3323.74	22	30077.96	
3293.29*	50	30356.00	$6g\,^2G_{11/2}$—$7h\,^2H^\circ_{11/2,\,13/2}$
3293.00*	45	30358.73	$6g\,^2G_{9/2}$—$7h\,^2H^\circ_{11/2}$
3133.32*	10	31905.76	$6f\,^2F^\circ_{7/2}$—$7g\,^2G_{9/2,\,11/2}$
3122.43*	10	32017.03	$6f\,^2F^\circ_{7/2}$—$7g\,^2G_{9/2}$
2301.48	30	43466.54	
2292.73	15	43602.75	$6p\,^2P^\circ_{3/2}$—$6d\,^2D_{3/2}$
2272.58	200	43989.27	$6p\,^2P^\circ_{3/2}$—$6d\,^2D_{5/2}$
2192.57	100	45594.40	$6p\,^2P^\circ_{1/2}$—$6d\,^2D_{3/2}$

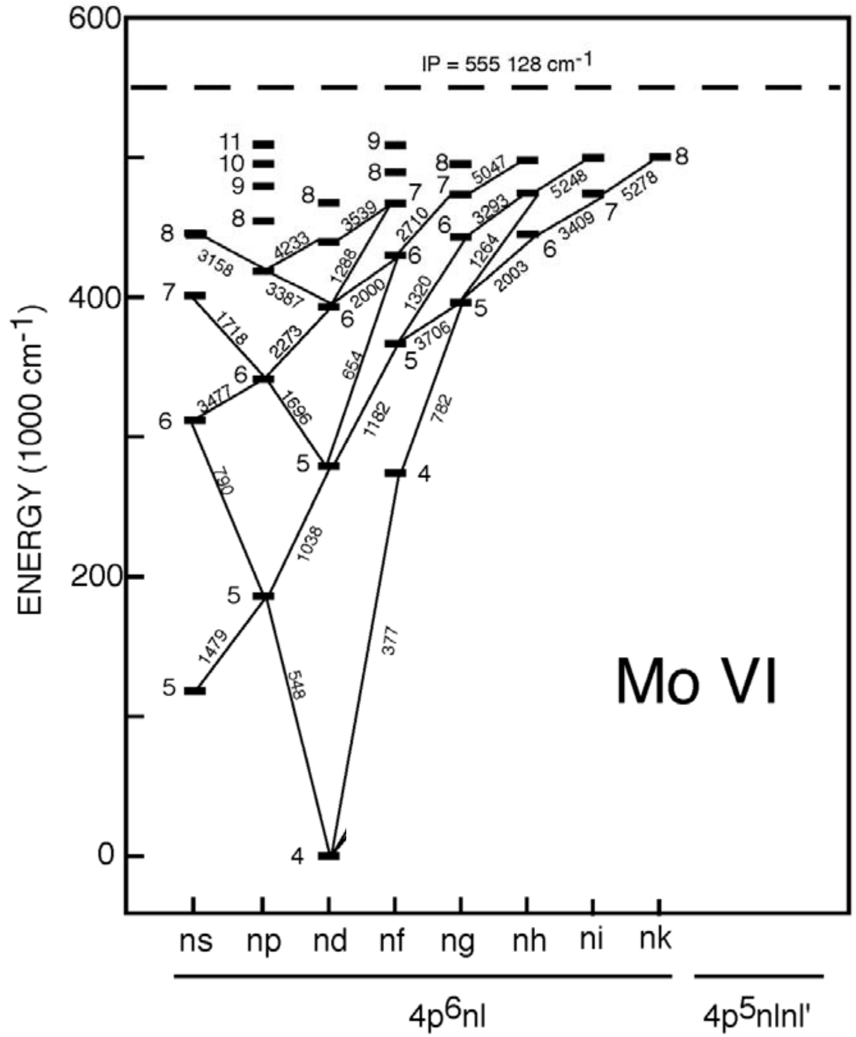
Table 2. Energy Levels of Mo VI

Configuration	Designation	J	Level, cm^{-1}	Interval
$4p^6(^1S)4f$	$4f\,^2F^0$	$2\frac{1}{2}$	$267043 + y$	409.62
		$3\frac{1}{2}$	$267452.62 + y$	
$4p^6(^1S)5d$	$5d\,^2D$	$1\frac{1}{2}$	$282821.36 + y$	785.36
		$2\frac{1}{2}$	$283606.72 + y$	
$4p^6(^1S)6s$	$6s\,^2S$	$\frac{1}{2}$	$313810 + x$	
$4p^6(^1S)6p$	$6p\,^2P^0$	$\frac{1}{2}$	$340573.85 + x$	1991.65
		$1\frac{1}{2}$	$342565.50 + x$	
$4p^6(^1S)6d$	$6d\,^2D$	$1\frac{1}{2}$	$386168.25 + x$	386.52
		$2\frac{1}{2}$	$386554.77 + x$	
$4p^6(^1S)7p$	$7p\,^2P^0$	$\frac{1}{2}$	$414856.35 + x$	1214.79
		$1\frac{1}{2}$	$416071.14 + x$	
$4p^6(^1S)7d$	$7d\,^2D$	$1\frac{1}{2}$	$439467.59 + x$	226.18
		$2\frac{1}{2}$	$439693.77 + x$	

ENERGY LEVELS OF ROMANOV AND STRIGANOV (1969)

Edlén, Tauheed, and Chaghtai (1985)

“Then a strong line at 2003 Å, slightly broadened by the unresolved splitting of 5g ^2G, could be definitely assigned to the transition 5g-6h which connects the chain of yrast levels 6h, 7i, and 8k to the rest of the term system.”



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ENERGY (1000 cm-1)
600
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0
ns
np
nd
nf
ng
nh
ni
nk
4p6nl
4p5nlnl'
Mo VI

	λ(air)					
	3122.43	10	32 017.03	(+2.5)	$7h\ ^2H - 9i\ ^2I$?	(RS)
	3133.32	10	31 905.76	0.0	$7i\ ^2I - 9k\ ^2K$	(RS)
	3293.00	45	30 358.73	0.0	$6g\ ^2G_{7/2} - 7h\ ^2H_{9/2}$	RS
	3293.29	50	30 356.00	0.0	$6g\ ^2G_{9/2} - 7h\ ^2H_{11/2}$	RS
	3323.74	22	30 077.96	0.0	$5f\ ^2F_{5/2} - 5g\ ^2G_{7/2}$	(RS)
	3343.20	1.5	29 902.89	0.0	$6d\ ^2D_{3/2} - 7p\ ^2P_{3/2}$	RS
	3386.98	20	29 516.39	0.0	$6d\ ^2D_{5/2} - 7p\ ^2P_{3/2}$	RS
	3408.60	200	29 329.11	0.0	$6h\ ^2H - 7i\ ^2I$	RS
	3476.60	200	28 755.50	0.0	$6s\ ^2S_{1/2} - 6p\ ^2P_{3/2}$	RS
	3484.77	13	28 688.10	0.0	$6d\ ^2D_{3/2} - 7p\ ^2P_{1/2}$	RS
OBS 3705.233 Å (INT=50,000)	(3705.34)				$5f\ ^2F_{7/2} - 5g\ ^2G_{9/2}$	
	3735.32	90	26 763.85	0.0	$6s\ ^2S_{1/2} - 6p\ ^2P_{1/2}$	RS
	4062.04	60	24 611.24	0.0	$7p\ ^2P_{1/2} - 7d\ ^2D_{3/2}$	RS
	4232.04	100	23 622.63	0.0	$7p\ ^2P_{3/2} - 7d\ ^2D_{5/2}$	RS
	4272.95	8	23 396.45	0.0	$7p\ ^2P_{3/2} - 7d\ ^2D_{3/2}$	RS
	5042.77	8.5	19 824.84	+0.1	$7g\ ^2G_{7/2} - 8h\ ^2H_{9/2}$	RS
	5043.55	10	19 821.77	0.0	$7g\ ^2G_{9/2} - 8h\ ^2H_{11/2}$	RS
	5247.45	35	19 051.57	0.0	$7h\ ^2H - 8i\ ^2I$	RS
	5276.86	45	18 945.40	0.0	$7i\ ^2I - 8k\ ^2K$	RS
	5448.82	7.5	18 347.51	0.0	$5f\ ^2F_{7/2} - 6d\ ^2D_{5/2}$	(RS)
	6035.62	0.75	16 563.72	0.0	$4f\ ^2F_{5/2} - 5d\ ^2D_{5/2}$	RS
	6188.67	11	16 154.10	0.0	$4f\ ^2F_{7/2} - 5d\ ^2D_{5/2}$	RS
	6336.04	5	15 778.36	−0.1	$4f\ ^2F_{5/2} - 5d\ ^2D_{3/2}$	RS

[a] For $\lambda > 3122$ Å the wavelengths are given in air and the intensity figures are copied from ref. [3]. Wavelengths in parentheses are predicted values.

[b] m = masked; b = broad line.

[c] Difference between predicted and observed wavenumber (cm^{-1}).

[d] Letters following the classification: C = identified by Charles [2]; T = identified by Trawick [1]; RS = measurement and identification by Romanov and Striganov [3]; (RS) = line from [3], new identification.

Rec 31 Dec 1985

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Tel. 046/12 46 20

15 Dec. 1985

Dear Joe,

This is to thank you very much for your encouraging letter. It did me a lot of good. I am improving but there is a long way to go.

Many thanks also for the collection of your recent papers which give so much new and important information on various spectra. I was specially interested in your results for sodium-like strontium which extends our knowledge of that sequence considerably. Concerning the polarization formula I have always emphasized that the second term has only a formal connection with quadrupole polarization. The formula is useful, however, for deriving series limits. This is confirmed, I think, by your experimental value for Sr^{27+} as compared to the value extrapolated on the basis of the polarization formula.

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With all good wishes to you and Evelyn from Friedel and myself,

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Physica Scripta. Vol. 16, 72–76, 1977

Energy Levels and Transition Probabilities in Mo XIV

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Department of Physics, University of Lund, Sölvegatan 14, S-223 62 Lund, Sweden

Received June 29, 1977

Abstract

Energy levels and transition probabilities in Mo XIV. L. J. Curtis, A. Lindgård, B. Edlén, I. Martinson and S. E. Nielsen (Department of Physics, University of Lund, Sölvegatan 14, S-223 62 Lund, Sweden). *Physica Scripta (Sweden) 16*, 72–76, 1977.

An investigation is made of the energy levels in Mo XIV (Cu I isoelectronic sequence). Published material is combined with previously unreported measurements to obtain reasonably accurate energies for terms with $n=4$, 5, 6, 7 and 8. For the ionization limit we find the value 2 441 ± 2 kK. These data are used to calculate transition probabilities, oscillator strengths and radiative lifetimes for a large number of transitions by means of a numerical Coulomb approximation procedure.

1. Introduction

In connection with spectroscopic studies of Tokamak discharges several authors [1, 2] have observed transitions in highly ionized molybdenum, in particular the $\Delta n=0$ resonance lines in Mo XIII, XIV, XXXI and XXXII (Zn, Cu, Mg and Na isoelectronic sequences, respectively). For diagnostic purposes it is of importance to determine the level structure and transition probabilities in these spectra.

In Mo XIV Hinnov [1] gives the wavelengths 423.5 ± 0.5 and 373.8 ± 0.5 Å for the $4s\ ^2S_{1/2}$–$4p\ ^2P_{1/2,3/2}$ doublet. These results can be combined with an earlier study in the XUV by Alexander et al. [3] who measured the wavelengths (to within ± 0.005 Å) of the $4s$–$5p$, $4s$–$6p$, $4p$–$5s$, $4p$–$5d$ and $4d$–$5f$ multiplets.

From refs. [1] and [3] we thus obtain the $4p\ ^2P$, $5p\ ^2P$, $6p\ ^2P$, $5s\ ^2S$ and $5d\ ^2D$ term energies. To determine the $4d\ ^2D$ and $5f\ ^2F$ energies only the $4d\ ^2D$–$5p\ ^2P$ wavelengths are needed. The spark spectrum of Mo has been recorded by one of us [4] and an extended analysis now gives the desired $4d$–$5p$ wavelengths as well as some additional $4s$–np, $4p$–ns and $4f$–ng transition wavelengths. By combining published measurements with our own determinations, wavelengths for transitions among fourteen different excited doublet terms were obtained. These data are listed as part of Table I, denoted according to their source by *a* (ref. [1]), *b* (ref. [3]) and *c*, *d* or *e* (our own measurements, of uncertainties ± 0.05, ± 0.1 or ± 0.2 Å respectively). These measured wavelengths were used to infer the term energies and ionization potential and to predict energies of additional terms using quantum defect expansions along various Rydberg series. The empirical set of term values so generated, although of uneven accuracy, permits the calculation of transition probabilities and oscillator strengths through the use of the Coulomb approximation with estimated uncertainties of ± 10% in this relatively simple spectrum.

2. Measurements

The measurements reported here are based upon two spectrograms, one in the region 35–121 Å and the other in the region 122–184 Å, which were recorded in Uppsala in 1937 using a 5-m grazing incidence spectrograph. The plate factor ranged from 0.28 Å/mm at the shorter wavelengths to 0.54 Å/mm at the longer wavelengths. The light source was a 0.4 μF, 60 kV vacuum spark between graphite rods, one of which was filled with Mo, the other with a mixture of Mo, BeO and B_2O_3, thus providing reference lines in Be, B and O. Two exposures were made, one for 1 hour 45 minutes, the other for 20 minutes.

Twelve Mo XIV multiplets were identified, ten of which were measurable in two fine structure components. In the cases of the $4p$–$5s$ and the $4d$–$5p$ multiplets the fine structure components with longest wavelength were beyond the end of the plate. This was particularly unfortunate for the case of the $4d$–$5p$, since it is vital to establishment of the $4d$ and $5f$ levels. It was possible to locate the weak $\Delta J=0$ satellite line, but this identification and wavelength measurement should be verified by a subsequent search for its other component at 185.0 Å. The results of our study confirmed the measurements of Alexander et al. [3] for the $4s$–$5p$, $4s$–$6p$, $4p$–$5s$, $4p$–$5d$ and $4d$–$5f$ transitions, and also included the $4s$–$7p$, $4p$–$6s$, $4p$–$7s$, $4p$–$8s$, $4f$–$5g$, $4f$–$6g$ and $4d$–$5p$ transition wavelengths. Since these plates were not originally taken with the aim of exclusively studying Mo XIV wavelengths, some of the lines needed in the present analysis were near the ends of the plates and not bracketed by reference lines. In such cases extrapolations rather than interpolations were needed. Thus some of the accuracies are below those usually reported in high resolution spectroscopic studies. However, they should be quite sufficient for plasma-diagnostic studies as well as for the calculation of transition probabilities to within present measurement accuracies.

3. Determination of the ionization potential and energy level extrapolations using quantum defect methods

The ionization potential was determined by a joint analysis of the $^2S_{1/2}$, $^2P_{1/2}$ and $^2P_{3/2}$ Rydberg series using a weighted non linear least squares minimizing parameter adjustment of the Ritz formula to the measured data. The procedure used is simple and general, and is described briefly below.

We denote the energy of a level with principal quantum number n, orbital angular momentum L and total angular momentum J by E_{nLJ}, and the uncertainty in its measurement by ΔE_{nLJ}. Our approach consists of searching for the value for E_∞, the ionization potential, which best allows the simultaneous description of all overdetermined Rydberg series by their respective Ritz formulae. For a given series the Ritz formula relates E_∞ to the measured E_{nLJ} through an expansion

$$\delta_{nLJ}(E_\infty) = a_{LJ} - b_{LJ} t_{nLJ}(E_\infty) + \dots \qquad (1)$$

in powers of t_{nLJ}, which is the term energy in units of the Rydberg energy R and the stage of ionization $\zeta - 1$

$$t_{nLJ}(E_\infty) \equiv (E_\infty - E_{nLJ})/R\zeta^2 \qquad (2)$$

[1] Permanent address: H. C. Ørsted Institute, University of Copenhagen, Universitetsparken 5, DK-2100 Copenhagen, Denmark.

Curtis, Lindgard, Edlen, Martinson, and Nielsen

"Published material is combined with previously unreported measurements to obtain reasonably accurate energies for terms with n=4, 5, 6, 7, and 8."

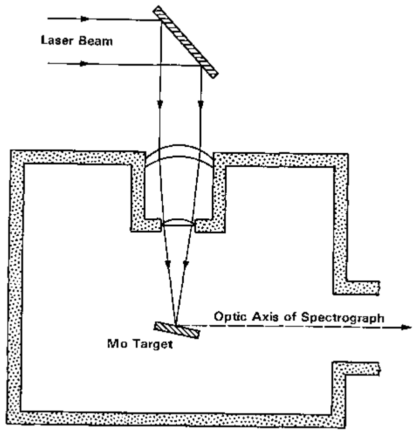


FIG. 1. Experimental arrangement for laser-produced plasma. The laser beam is about 2 cm in diameter. The target is inclined toward the spectrograph at an angle of about 5°.

rectly with the stage of ionization. These line width observations are more fully described in Ref. 4.

ANALYSIS OF THE SPECTRUM

In the first stage of the analysis, we combined our measurements of the $4s$-$4p$ resonance lines with the identifications of Alexander *et al.*[1] to construct a system of levels containing the $4s$, $4p$, $5s$, $5p$, $5d$, $5f$, and $6p$ configurations. A plot of the energy levels and observed lines of Mo XIV is shown in Fig. 2.

We then considered the $4d$ configuration. The $4p$-$4d$ transitions were predicted by Weiss[16] to lie in the region around 250 Å, which is extremely dense in the spark spectrum and also fairly complicated in the laser-produced spectrum. We therefore turned to the $4d$-$5p$ transitions, expected at about 180 Å. This is a much simpler region in the spark spectrum and extremely simple in the laser-produced spectrum. A portion of the spectrum in this region is reproduced in Fig. 3. As shown, all three of the $4d$-$5p$ transitions of Mo XIV can be identified readily. The $5p$ ^{2}P interval of 13 227 cm^{-1} implied by these identifications agrees well with the interval of 13 203 cm^{-1} given by the $4s$-$5p$ transitions at 83 Å.

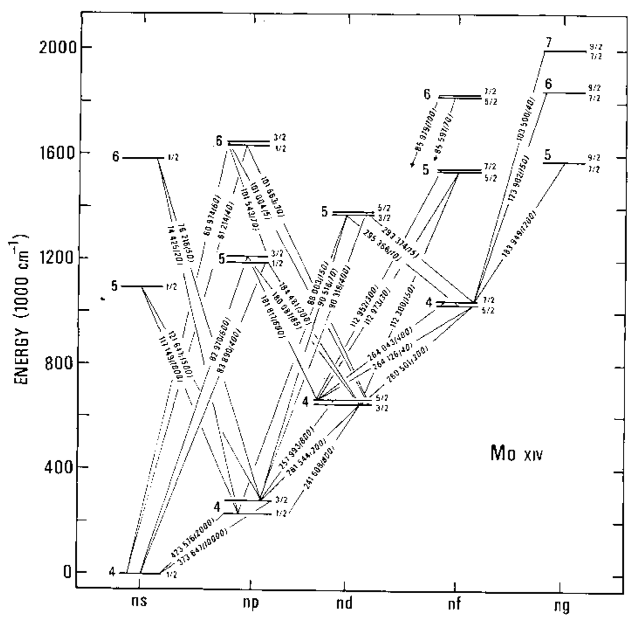


FIG. 2. Grotrian diagram for Mo XIV. Wavelengths are in Å. Intensities are indicated in parentheses following the wavelengths. Wavelengths for the $4s$-$5p$, $4s$-$6p$, and $4p$-$5d$ transitions are those calculated from the optimized level values.

Reader, Luther, Acquista (1979)

Spectrum and energy levels of thirteen-times ionized molybdenum (Mo XIV)

Joseph Reader, Gabriel Luther, and Nicolo Acquista
National Bureau of Standards, Washington, D.C. 20234
(Received 27 June 1978)

The spectrum of Mo XIV was observed with a low-inductance spark and a laser-produced plasma in the region from 70 to 630 Å on the10.7-m grazing-incidence spectrograph at NBS. From the identification of 35 lines, a system of 22 energy levels was determined. The level system (Cu I isoelectronic sequence, $3d^{10}nl$) includes the series ns (n = 4–6), np (n = 4–6), nd (n = 4,5), nf (n = 4–6), and ng (n = 5–7). The observed energy levels are compared with Hartree-Fock calculations. The ionization energy is determined from the ng series (n = 5–7) to be 2 440 600 ± 300 cm^{-1} (302.60 ± 0.04 eV).

The spectra of highly ionized molybdenum atoms have been of considerable interest lately because of their appearance in controlled thermonuclear research plasmas. The Mo XIV ion is especially useful for plasma diagnosis because it has a simple spectrum, with the total emitted intensity concentrated in just a few lines.

Mo XIV is a member of the Cu I isoelectronic sequence; the ground configuration is $3d^{10}4s$, and the excited configurations are all of the type $3d^{10}nl$. In 1971, Alexander, Even-Zohar, Fraenkel, and Goldsmith[1] observed the spectrum of Mo XIV in the region from 45 to 350 Å with a low-inductance spark and identified the strong $4s$-$5p$, $4s$-$6p$, $4p$-$5s$, $4p$-$5d$, and $4d$-$5f$ transitions. In 1972, Hinnov, Johnson, Meservey, and Dimock[2] observed the $4s$-$4p$ resonance doublet (373 and 424 Å) in the Princeton ST tokamak and measured the wavelengths to an accuracy of ± 1 Å. In 1976, Hinnov[3] measured these lines to an accuracy of ± 0.5 Å.

Recently two of us[4] observed the $4s$-$4p$ resonance lines of the six copper-like atoms Rb IX - Mo XIV in a low-inductance spark. These observations confirmed the identification of the Mo XIV lines in tokamak plasmas.[2,3] In the present paper we report our complete observations and energy levels for Mo XIV.

As the present work was nearing completion, a paper on Mo XIV by Curtis, Lindgård, Edlén, Martinson, and Nielsen[5] appeared. This paper reports the observation of the Mo XIV spectrum with a high-voltage spark in the region from 35 to 184 Å. Identifications are given for the $4s$-$7p$, $4p$-$6s$, $4p$-$7s$, $4p$-$8s$, $4f$-$5g$, $4f$-$6g$, and $4d$-$5p$ transitions, with wavelengths ranging in accuracy from ±0.05 to ±0.2 Å. By combining these measurements with those in Refs. 1 and 3, a set of twenty-nine energy levels was obtained. Nineteen of the level values in this set were derived directly from observed lines; ten were deduced from semiempirical considerations. In comparing the present results with those in this paper we find that our $4p$-$6s$ line identifications are the same. However, our $4d$-$5p$, $4f$-$5g$, and $4f$-$6g$ identifications are different. The energy level systems thus differ considerably.

EXPERIMENT

The spectra were excited in two different light sources. The first was a low-inductance open spark, essentially the same as described by Feldman, Schwartz, and Cohen.[6] In this source the spark takes place between metallic electrodes in vacuum after being triggered by a high-frequency discharge from a third electrode. In the present work we used capacitors of either 4.7 or 14.2 μF at voltages varying between 1 and 15 kV.

The second source was a laser-produced plasma. This was obtained by focussing the light from a Nd/glass laser (wavelength 1.06 μm) onto a flat metallic target. The focussing lens was a two-component system having an effective focal length of about 70 mm. The geometrical arrangement is shown schematially in Fig. 1. The diameter of the focal spot at the target was about 200 μm. Typical laser pulses had an energy of 15 J and a duration of 10 ns.

The spectra were recorded on our 10.7-m grazing-incidence spectrograph. The grating had 1200 lines/mm, providing a plate factor of 0.25 Å/mm at 300 Å. The angle of incidence was 80°. At this angle the lowest wavelength that could be observed was about 70 Å; the highest was 630 Å.

Wavelength calibration in the region around 100 Å was obtained from a low-inductance spark of Ti.[7] In higher regions calibration was obtained from internal lines of Mo VII–IX[8–10] and impurity lines of oxygen and fluorine.[11–15] Most of the Mo lines around 100 Å were also measured in the 2nd and 3rd orders. No shifts of wavelength with order were detected.

The ionization stages of the observed lines were distinguished in several ways. First, the spectra were compared with spectra taken with a low-voltage sliding spark. Our previous work[10] showed that the sliding spark would not produce atoms of Mo ionized more than about eight times. Second, the variation of line intensity with spark voltage was observed. We found that the spectrum of Mo XIV was not significantly excited at voltages below 3 kV and showed practically no enhancement at voltages above 3 kV. Third, the spectrum of the low-inductance spark was compared with the spectrum of the laser-produced plasma. The laser-produced spectrum was much simpler than the spark spectrum because it did not contain spectra of ions below Mo X. We also found that with the laser-produced plasma the spectrum of Mo XIV could be enhanced relative to spectra of higher stages of ionization by using laser pulses of greater energy and longer duration, typically 30 J in 20 ns. Finally, in the long wavelength region of the spark spectra, lines belonging to higher ionization stages could be recognized by their relatively large widths. In general the observed line widths varied di-

READER, LUTHER, ACQUISTA (1979)

"…a paper on Mo XIV by Curtis, Lindgard, Edlén, Martinson, and Nielsen appeared…

…our 4p-6s line identifications are the same. However, our 4d-6p, 4f-5g, and 4f-6g identifications are different. The energy level systems thus differ considerably."

Dr.A.N.Ryabtsev
Institute for Spectroscopy
USSR Academy of Sciences
Troitsk, Moscow Region 142092
USSR

Prof. B.Edlén

Physics Department
University of Lund
S-223 62 Lund
Sweden

November 13, 1985

Dear Prof. Edlén:

In continuation of our work on autoionizing states (Physica Scripta 1984,30,407) we transferred our attention to the Rb I sequence. The idea was to look at the levels of $4p^5 4d5s$ configuration in Y III - Mo VI. M.Chaghtai et al claimed their identification (J.Phys.B, 1979,12,19). But the very first spectra of Nb and Mo in the region $\lambda < 300$ Å taken in favorable conditions for excitation of Nb V and Mo VI showed that Chaghtai's analysis may not be considered as serious. For example in Mo VI out of 27 suggested lines only 10 ones could belong to this stage of ionization but their identification with the $4p^6 4d - 4p^5 4d5s$ transitions is questionable.

With a great sorrow I have bad news also for one-elrctron spectrum of Mo VI wich is under publication by M.Chaghtai et al with your participation (many thanks for the manuscript before publication). Identification of 4d - 6f transitions is certainly incorrect as well as the location of 8p levels. In our spectrum 4d - np and 4d - nf series can be traced up to n=11 and 9 respectively. The line 232.801 Å of the manuscript is too weak for 4d - 6f transition and 233.457 Å is in fact O IV line. We found three other lines (229.266 [3/2-5/2], 230.437 [5/2-7/2] and 230.633 [5/2-5/2] Å) wich undoubtely represent these transitions. Similarly our spectrum does not have lines 4d - 8p on predicted places. Instead, $8p_{3/2}$ level must be placed at 456713 cm^{-1} and $8p_{1/2}$ at 456491 cm^{-1} (there is other choise for this level: 455807 cm^{-1}, but less probable). The energies of these

Ryabtsev letter to Edlén (1985)

"With a great sorrow I have bad news also for one-electron spectrum of Mo VI which is under publication by M. Chaghtai et al with your participation (many thanks for the manuscript before publication). Identification of 4d-6f transitions is certainly incorrect as well as the location of the 8p levels."

series are listed below:

	8p	9p	10p	11p
1/2	456491?	481359?	498024	509597
3/2	456713	481762	498228	509779
	6f	7f	8f	9f
5/2	436174	467823	488710	502976
7/2	436542	467938	488750	502996

The values are preliminary and may be changed on a couple of cm^{-1} after final averaging. The analysis of $\delta - (n^*)^{-2}$ plot for these series suggests that ionization limit might be not accurate. If so than it casts doubts on identification of 6h, 7i and 8k levels used for deriving the limit.

Sorry once more. Hope the information will have some value for you.

Yours sincerely

A.N. Ryabtsev

A.N.Ryabtsev

COPY #2 # 11030

Lithuanian Physics Journal, V. 31, No. 3, 143 — 149, 1991

Atoms and molecules

Highly excited configurations in the spectrum of Mo VI

A. Kancerevicius

(Institute of Theoretical Physics and Astronomy, Lithuanian Academy of Sciences)

A. Ramonas

(Lithuanian Science Society)

A.N. Ryabtsev and S.S. Churilov

(Institute of Spectroscopy, Academy of Sciences of the USSR)

Received 17 September 1990

UDC 539.182; 539.184.2

More than 100 spectral lines of Mo VI have been identified in the wavelength region 196 – 352 A. Previous analysis of the $4p^64d - 4p^54d^2$ and $4p^64d - 4p^54d5s$ transitions has been revised. 37 out of 45 levels of the $4p^54d^2$ configuration and 20 out of 23 levels of the $4p^54d5s$ configuration have been found. Also energies of levels in the series of one-electron excitation $4p^6np$ ($n = 8 \ldots 11$) and $4p^6nf$ ($n = 4 \ldots 7$) have been determined. The analysis of spectra has been based on semiempirical calculations of the interacting configurations $4p^54d^2 + 4p^54d5s + (6 \ldots 8)p + (4 \ldots 7)f$.

The problem of the investigation of spectra of the molybdenum ions of all ionization degrees was put forward nearly 10 years ago so as to supply the studies on the controled thermonuclear fusion in "Tokamak" type facilities with the spectral data. More or less complete data on energy levels of all molybdenum ions are nowdays available [1]. At present extension of the studies of the energy structure of ions, a critical analysis of the accessible data, increase of their reliability become vitally important.

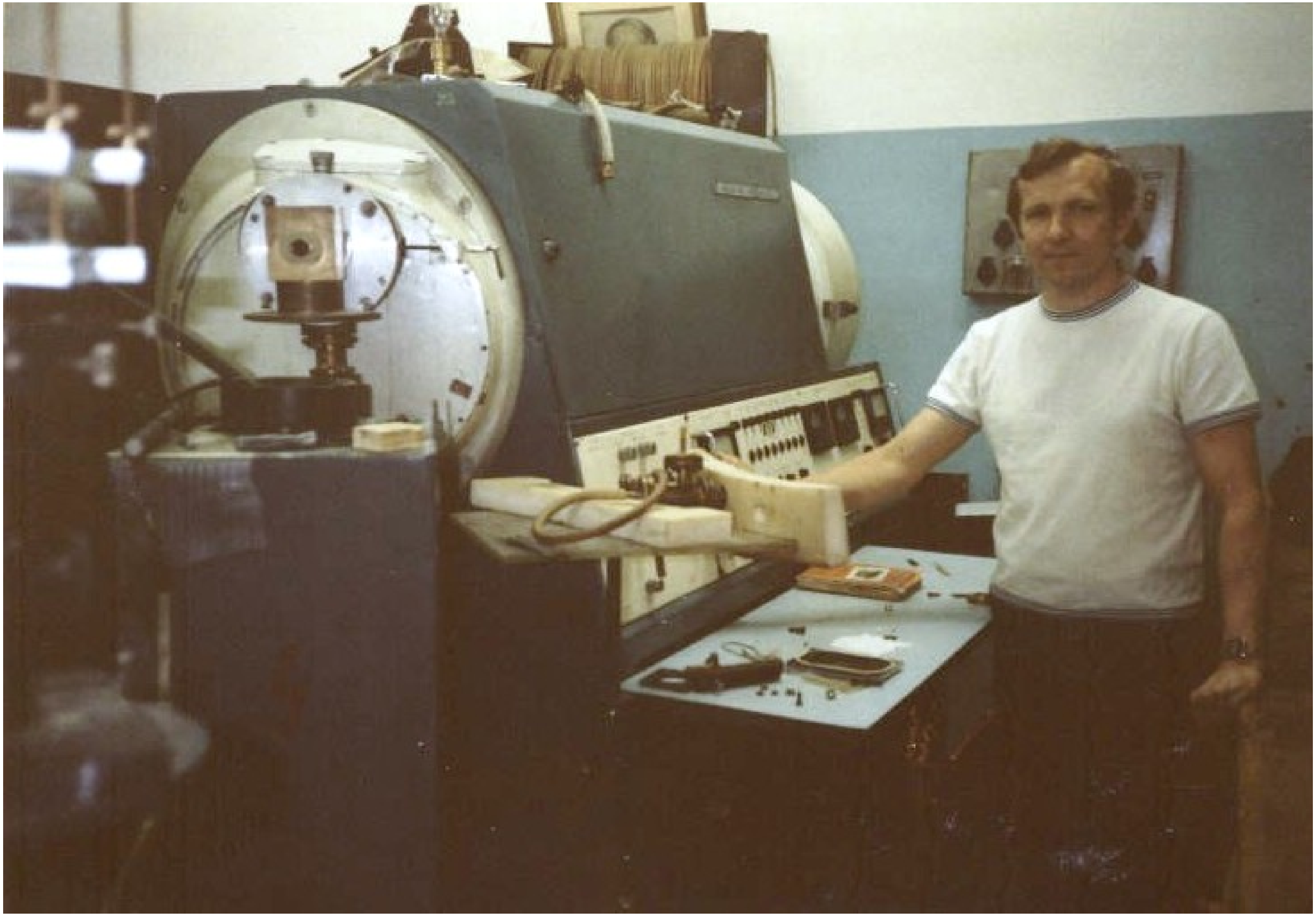
Recently, sufficiently great attention has been paid to the spectrum of Mo VI. Mo VI belongs to the rubidium isoelectronic sequence and has the ground state $4p^64d$. Observations in the *Alkator A* tokamak plasma [2] have confirmed the previous identification [3] of the one-electron transitions $4d - 5p$ and $4d - 4f$. Later on the one-electron spectrum was studied in detail in [4], where the one-electron configurations $4p^6nl$ with l varying from s to k and n reaching 9 were found. By means of extrapolation from the Ru VIII – Pd X [5] ions, the transitions $4p^64d - 4p^54d5s$ were identified, and the data on the configuration with the excitation of the inner electron $4p^54d5s$ were obtained [6]. Paper [7] reports the studies of another configuration with the inner electron excitation, namely that of $4p^54d^2$. Below are presented the results of the analysis of the Mo VI spectrum in the region < 350 A, where the transitions from highly excited states, including the $4p^54d5s$ and $4p^54d^2$ configurations, are located. Owing to high resolution, a sufficiently good distinguishing of a majority of the Mo VI lines from the sum total of lines, which belong to other ionization degrees, as well as to the application of the semiempirical procedure of the spectrum calculation, the data on the one-electron spectrum have been expanded towards large n, the classification of the transitions $4p^64d - 4p^54d^2$, $4p^54d5s$ has been revised and corrected. Certain errors in the previous identification of the one-electron spectrum have been removed. The preliminary results, concerning some Mo VI energy levels, were presented at the SASHIA Conference [8] and were included into the compilation of the USA National Bureau of Standards [9].

The Mo VI spectrum has been excited in the three electrode vacuum spark in the low inductance spark chamber. Two spark regimes have been adopted to distinguish between lines in accordance with ionization degrees: hot, for which $C = 12\,\mu F$, $L = 0.6\,\mu H$, $U = 4$ kV, $I_{max} = 14$ kA, and cold, for which $C = 7500\,\mu F$, $L = 3.8\,\mu H$, $U = 220$ V, $I_{max} = 1.5$ kA. The discharge form was close to the regime of the critical damping. For this pur-

KANCEREVICIUS, RAMONAS, RYABTSEV, CHURILOV (1991)

“Analysis of our spectra shows that the energies of both 6f and 8p upper configurations in [4] (Edlén et al.) are erroneous”

“On account of what has been stated above it is obvious that a revision of the identification of the transitions between highly excited states of Mo VI in the long wavelength region carried out in [4] is desirable. The errors in determining the energies of the levels 6f and 8p lead to the erroneous identification of the transitions 5d-8p, 5d-6f, 6s-6p, 6d-6f, 6f-7g. This, in its turn, brings about doubts as to the identification of both the transition 7g-8h as well as of the obtained value of the Mo VI ionization potential.”



A. N. Ryabtsev and 3-m grazing-incidence spectrograph (1983)

S. S. Churilov repairing vacuum pump (1983) from Litzén   16 May 1989

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          necessarily be returnable through this path.
From:     General Delivery <POSTMASTER@SELDC52>
Subject:  TO JOE FROM ULF
To:    JOSEPHREADER@CSCS855.CS2
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Dear Joe,

Thanks for your letter and our best wishes and congratulations to the happy Grandparents. Hope you had a good time in California.

I mailed the reprints of our Ge-like paper some time ago - I suppose you will receive them any day now.

The direct reason for this message is to warn you that I will call you soon, maybe already today, on behalf of Bengt Edlen. He is rather worried about the analysis of Mo VI, where he, as you know, is a co-author with Chaghtai and some other Indians. The reason for his worries is that Ryabtsev has pointed out that there are some errors in the analysis, and he wants to know how serious it is. I told him that you might have some information on this, as you are working on Mo VII. To be more specific, Ryabtsev has questioned 6f, 8p and the ionization limit. That does not sound too serious to me, but Bengt is worried.

Don't put any work into this now, I will just call and ask for your opinion if something should be done, and if it then could be done with your material.

Sincerely
Ulf

He is rather worried about the analysis of Mo VI, where he, as you know, is a co-author with Chaghtai and and some other Indians. The reason for his worries is that Ryabtsev has pointed out some errors in the analysis, and he wants to know how serious it is. I told him that you might have some information on this, as you are working on Mo VII. To be more specific, Ryabtsev has questioned 6g, 8p, and the ionization limit. This does not sound too serious to me, but Bengt is worried.

Don’t put any work into this now, I will just call and ask for your opinion if something should be done, and if it then could be done with your material.

Sincerely

Ulf

EXPERIMENT AT NIST – new plates 1996

LIGHT SOURCE

SLIDING SPARK DISCHARGE

Mo electrodes with quartz spacer

Peak currents 300 – 2300 A

Excellent separation of stages of ionization

SPECTROGRAPHS

10.7-m GRAZING-INCIDENCE

150 – 500 Å

10.7-m NORMAL-INCIDENCE

400 – 5300 Å

CALIBRATION

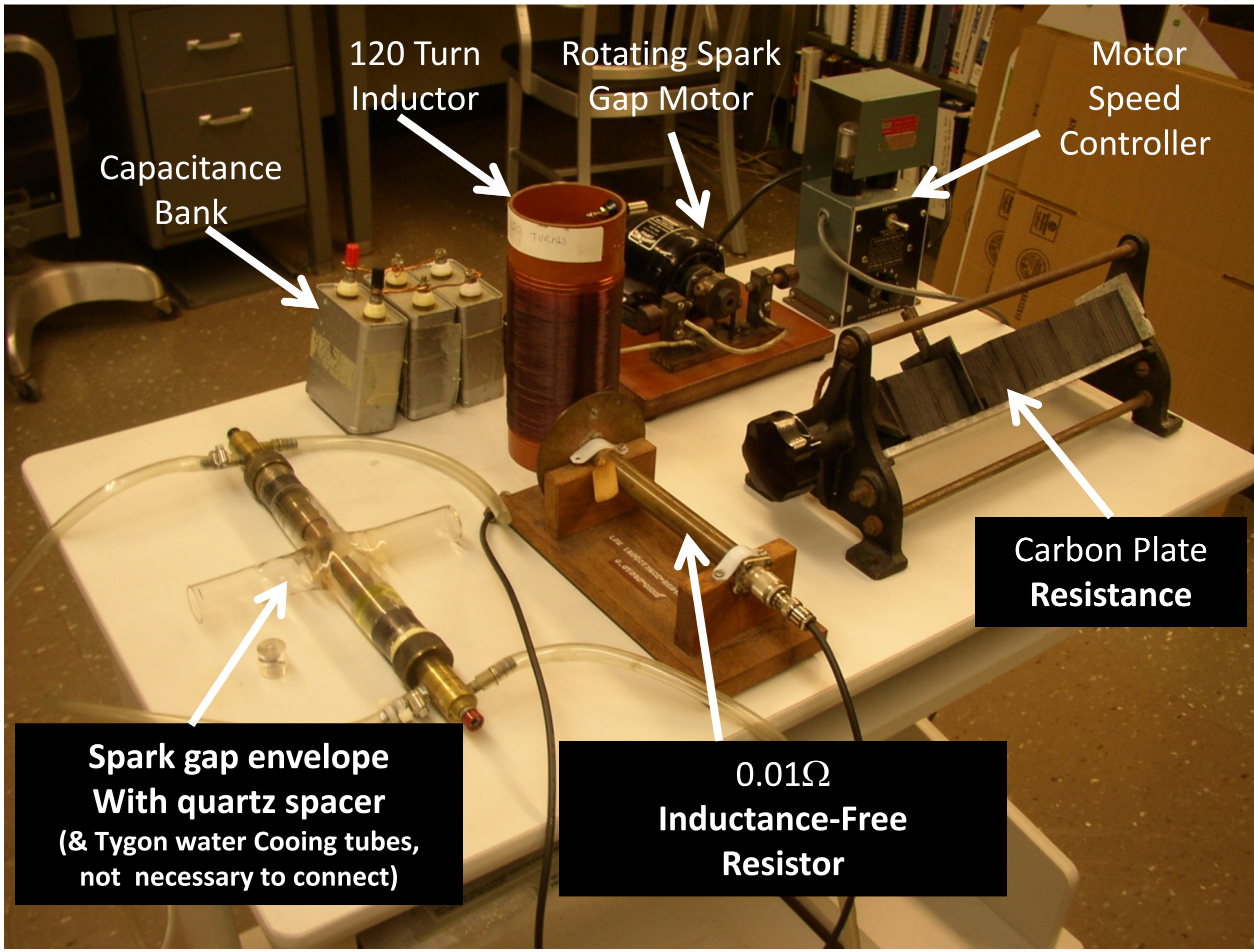
Y SLIDING SPARKS

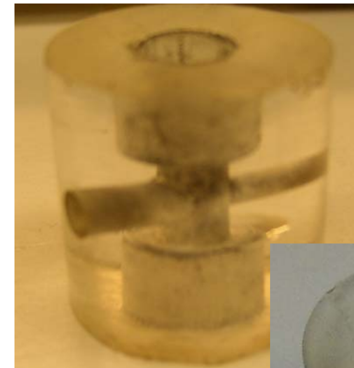
Platinum hollow cathode

Thorium hollow cathode

ACCURACY

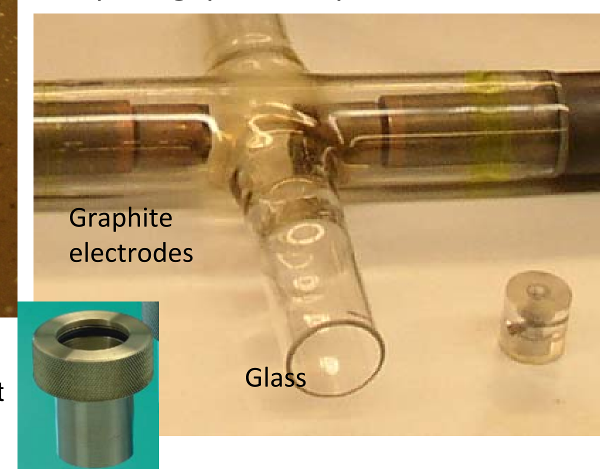
Wavelength uncertainty: ± 0.005 Å






Quartz Spacer

Spark gap envelope



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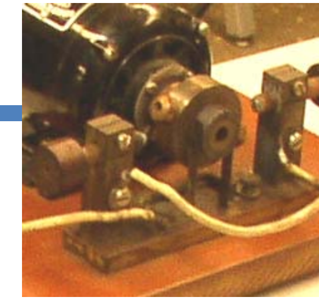
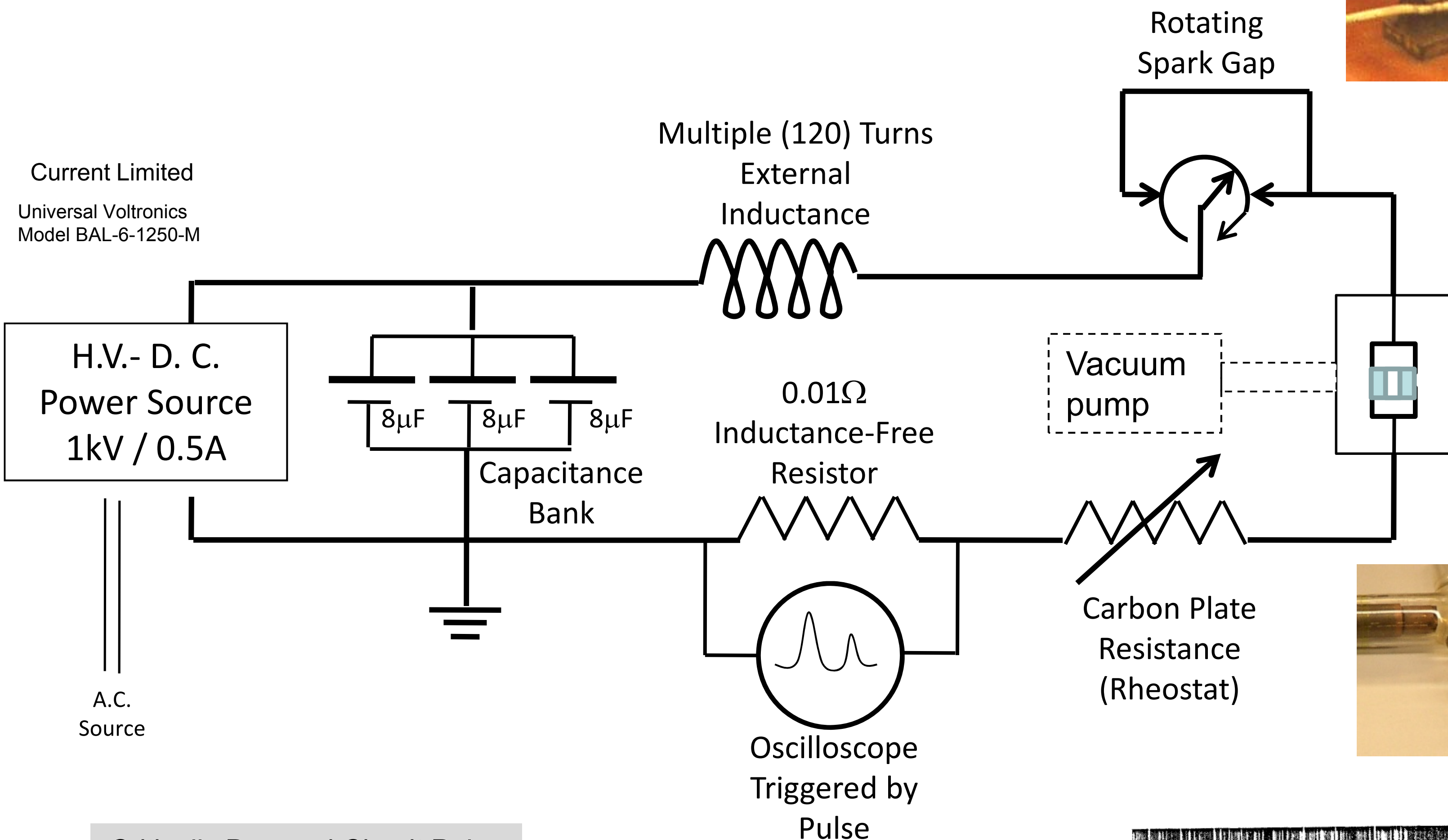
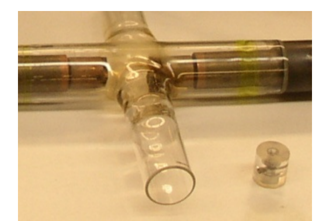
Universal Voltronics Model BAL-6-1250-M
(Alternate: EMI TCR1500S1.5-2-1202; **SPEC3211A**)

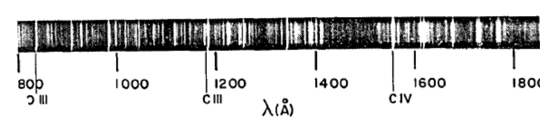




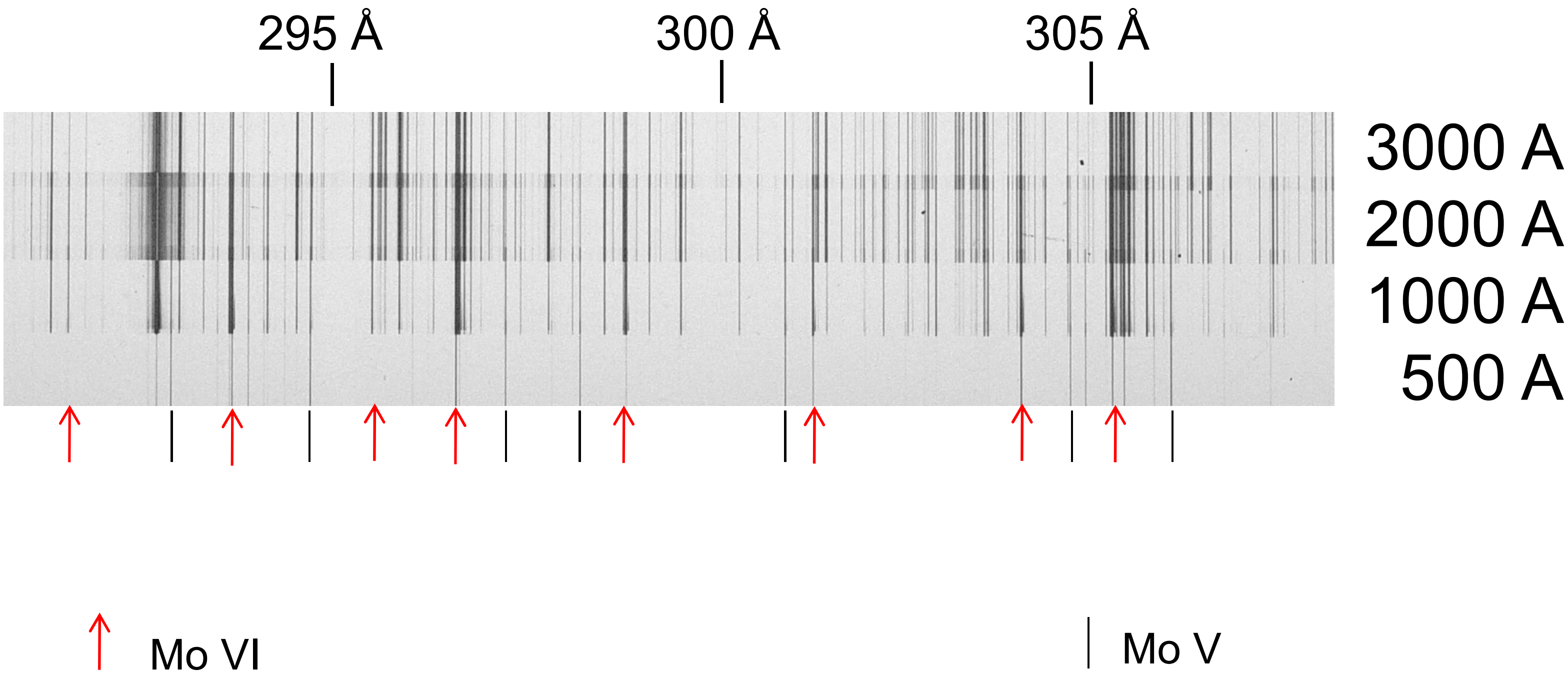


Critically Damped Circuit Pulse

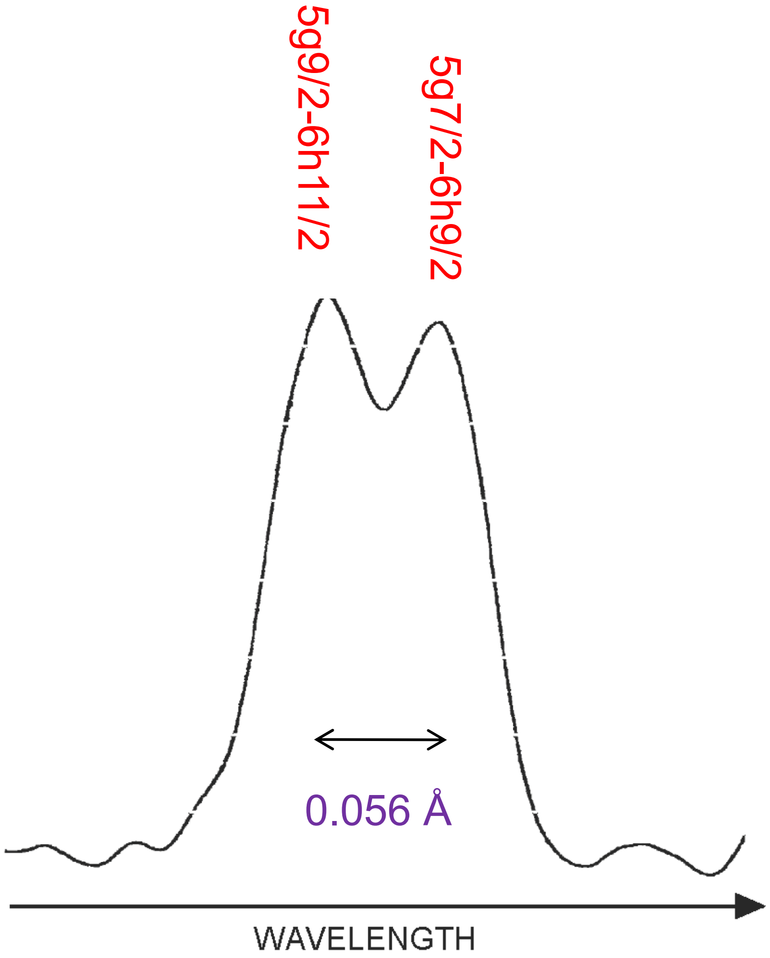
$R^2=4L/C \quad t\sim L/R$



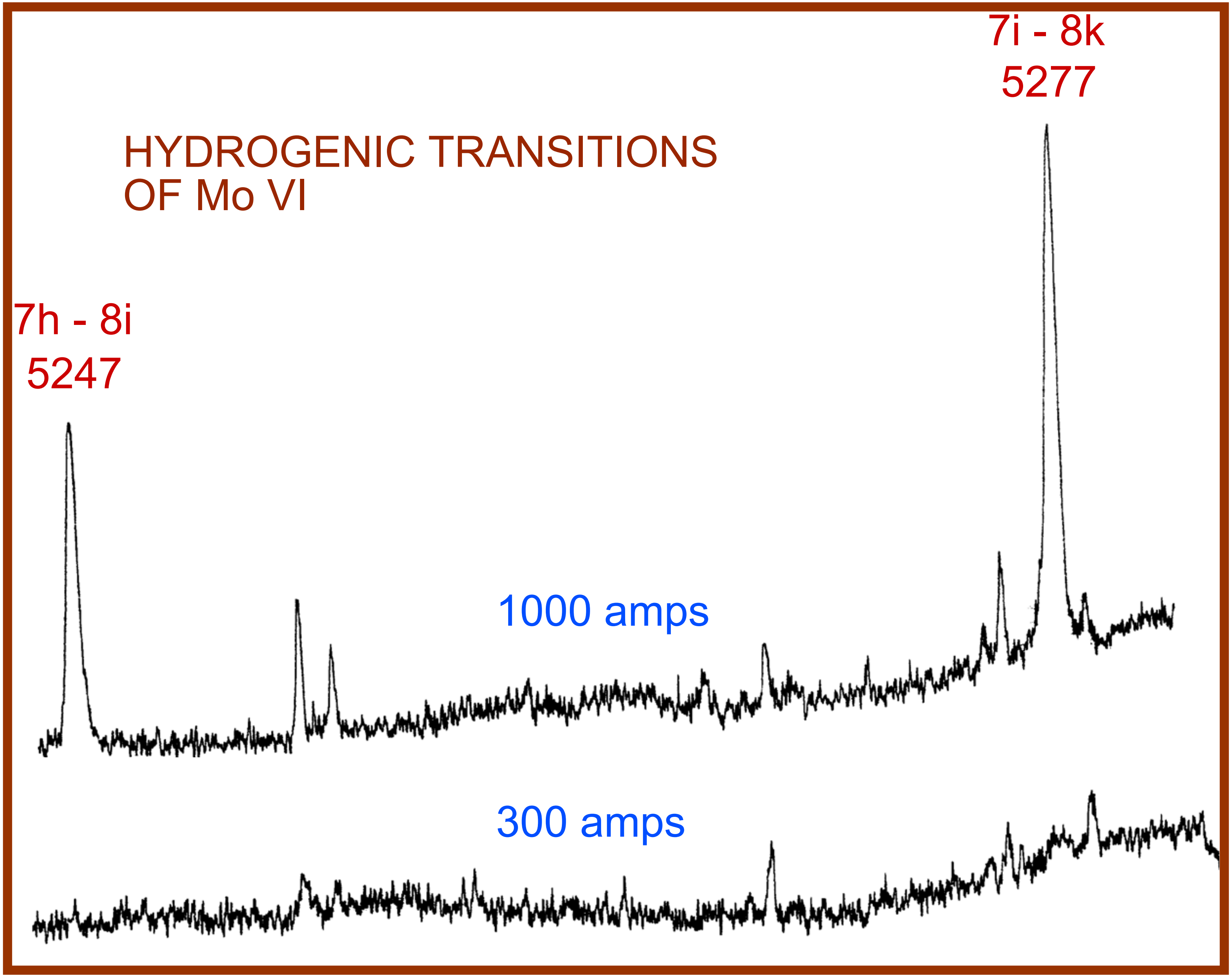
Al,Spark-excited

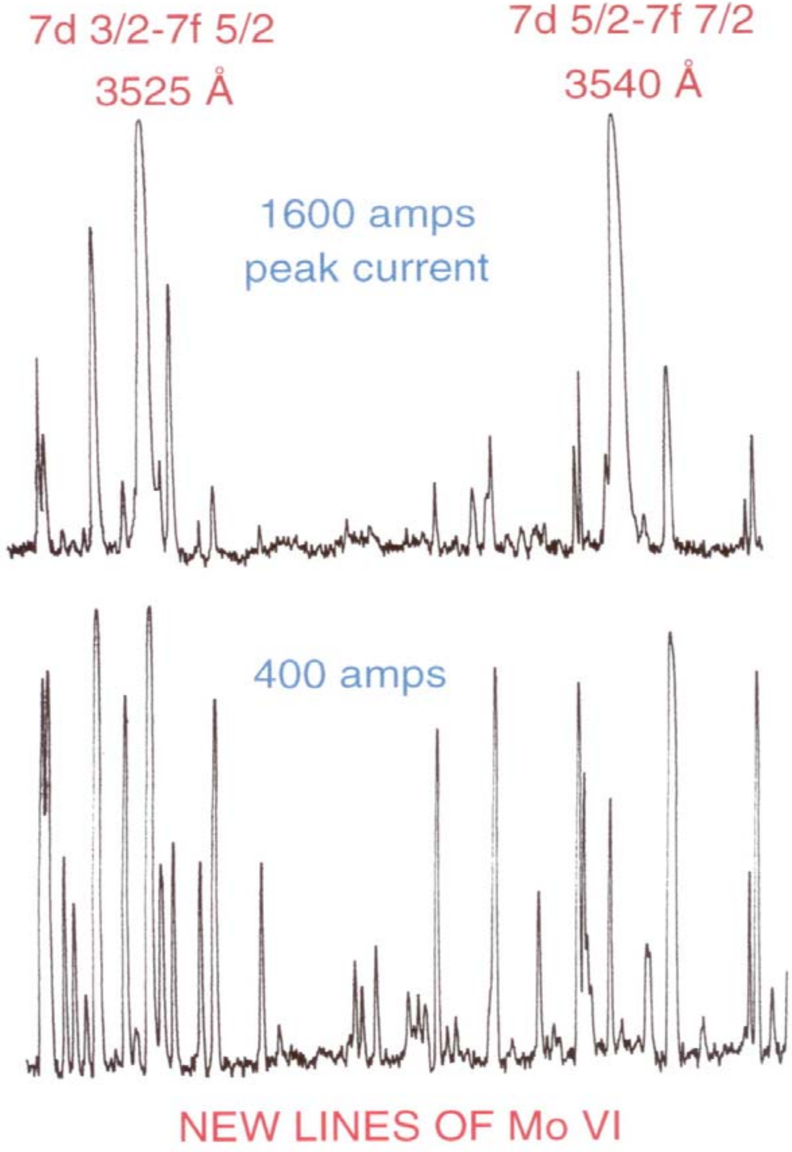


SLIDING SPARK SPECTRA OF Mo on 10.7-m GRAZING-INCIDENCE SPECTROGRAPH



2003 Å line of Mo VI


7i - 8k
5277
HYDROGENIC TRANSITIONS
OF Mo VI
7h - 8i
5247
1000 amps
300 amps


7d 3/2-7f 5/2
3525 Å
7d 5/2-7f 7/2
3540 Å
1600 amps
peak current
400 amps
NEW LINES OF Mo VI

RESULTS

- IMPROVED WAVELENGTHS: 200-5300 Å – 234 lines total
- IDENTIFICATIONS FOR PENNING LINES
- NEW LINES FOR HIGH LEVELS
- REVISED EVEN-PARITY LEVELS OF EDLÉN
- REVISED A FEW KANCEREVICUIS IDENTIFICATIONS
- 112 ENERGY LEVELS TOTAL
- SLIGHT REVISION OF IONIZATION ENERGY
- ACCURATE RITZ-TYPE WAVELENGTHS

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Spectrum and energy levels of five-times ionized molybdenum, Mo VI

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Abstract

The Mo VI spectrum was photographed with a sliding spark discharge on the 10.7 m normal-incidence and grazing-incidence vacuum spectrographs at the National Institute of Standards and Technology. The observations covered the region 196–5300 Å. The existing analysis of this spectrum due to Edlén *et al* (1985 *Phys. Scr.* **32** 215) and Kancerevicius *et al* (1991 *Lith. Phys. J.* **31** 143) was revised and extended. The ionization energy of Edlén *et al*, which had been called into question by Kancerevicius *et al*, was confirmed. There are now a total of 234 lines and 112 energy levels. From the optimized energy levels, Ritz-type wavelengths with uncertainties varying from 0.0003 to 0.0018 Å were determined. The energy levels were theoretically interpreted by means of Hartee–Fock calculations and least-squares fits of the energy parameters to the observed levels. The fitted energy parameters were used to calculate oscillator strengths for all observed lines. By applying a polarization formula to the 6h–8h, 7i–8i, 8k levels, a revised value of the ionization energy of 555 127.5 ± 1.7 cm^{-1} (68.827 03 ± 0.000 21 eV) was determined.

1. Introduction

Five-times ionized molybdenum is a member of the rubidium isoelectronic sequence. The ground configuration is $4p^64d$. Excited configurations are of the type $4p^6nl$ and $4p^5nln'l'$. Following the first assignments for the 4d, 5s, 5p, 5d and 6s configurations by Trawick [1], Charles [2] reported assignments for the 4f and 6p configurations. His 6p assignments were later found by Romanov and Striganov [3] to be spurious. The results of Trawick and Charles were summarized in the compilation of energy levels by Moore [4]. Romanov and Striganov [3] used a high-current Penning discharge to observe the spectrum from 2192 to 6336 Å. They identified a number of lines as nl–nl' transitions, some with principal quantum number and orbital angular momentum as high as 8k. Level values could not be determined for all the identified lines, because some of the lower levels were not connected to the ground state.

Edlén *et al* [5] used spark light sources to observe the spectrum from 230 to 2350 Å. They extended the level system to include the 5s–8s, 4d–8d, 4f–6f, 5g–8g, 6h–8h, 7i–9i and 8k–9k configurations. The higher angular momentum states were based on the identifications of Romanov and Striganov [3]. Edlén *et al* [5] connected these states to the main system of levels by identifying a line at 2003 Å as the (unresolved) 5g–6h multiplet. They derived an ionization energy by fitting the 6h, 7i and 8k levels to a polarization formula.

Transitions involving inner-shell excitations have had several previous investigations. Mushtaq *et al* [6] identified $4p^64d$–$4p^54d5s$ transitions from observations in the region 191–238 Å and reported 19 energy levels of $4p^54d5s$. Tauheed *et al* [7] identified $4p^64d$–$4p^54d^2$ transitions from observations in the region 238–346 Å and reported 38 energy levels of $4p^54d^2$. They pointed out the strong interaction between the levels of $4p^54d^2$ and $4p^6nl$ levels and identified a number of transitions between $4p^54d^2$ and $4p^6nl$ levels, normally forbidden as two-electron jumps, extending to 2520 Å.

Kancerevicius *et al* [8] used a novel three-electrode spark, termed a 'semi-sliding vacuum spark', to observe the spectrum in the region 196–352 Å. They identified more than 100 lines of the types 4d-np, 5s-np, 4d-nf, $4p^64d$–$4p^54d5s$ and $4p^64d$–$4p^54d^2$. For the $4p^54d5s$ energy levels, only four levels of Mushtaq *et al* [6] were confirmed. For the $4p^54d^2$ energy levels, only five levels of Tauheed *et al* [7] were confirmed. Kancerevicius *et al* [8] further noted that the 6f and 8p levels of Edlén *et al* [5] were in error. They stated: 'The errors in determining the energies of the levels 6f and 8p lead to the erroneous identification of the transitions 5d–8p, 5d–6f, 6s–8p, 6d–6f, 6f–7g. This, in its turn, brings about doubts as to the identification of both the transition 7g–8h as well as of the obtained value of the Mo VI ionization potential.'

Table 1. Observed spectral lines of Mo VI. All wavelengths are in vacuum.

Wavelength (Å)					Wave	Even	Odd		
Present	Previous	Ref[a]	Intensity[b]		number (cm^{-1})	level[c]	level[c]	gA (s^{-1})	Log (gf)
196.234	.233	K	4		509 596	4d3	11p1	1.29×10^{9}	2.13
197.160	.163	K	5		507 202	4d5	11p3	2.16×10^{9}	−1.90
198.	.817	K	50		502 976	4d3	9f5	2.01×10^{10}	−0.92
199.828	.835	K	80		500 430	4d5	9f7	3.14×10^{10}	−0.73
200.788	.794	K	8		498 038	4d3	10p1	1.84×10^{9}	−1.95
201.729	.733	K	15		495 715	4d5	10p3	3.14×10^{9}	1.72
204.619	.620	K	100		488 713	4d3	8f5	3.37×10^{10}	−0.68
205.690	.691	K	150		486 169	4d5	8f7	5.33×10^{10}	−0.47
207.752	.745	K	8	u	481 343	4d3	9p1	2.88×10^{9}	−1.73
208.692	.691	K	60		479 175	4d5	9p3	5.04×10^{9}	−1.48
213.018	.017	K	90		469 444	4d3	ps75	1.73×10^{9}	1.93
213.755	.756	K	1 000		467 825	4d3	7f5	6.81×10^{10}	−0.33
214.195	.196	K	1 000		466 864	4d5	ps75	3.52×10^{10}	0.62
214.407	.409	K	200		466 403	4d3	ps63	5.49×10^{9}	−1.42
214.888	.890	K	1 500		465 359	4d5	7f7	1.13×10^{11}	−0.11
214.942	.942	K	110		465 242	4d5	7f5	5.88×10^{9}	1.39
215.598	.600	K	2 500	dc	463 826	4d5	ps47	8.51×10^{10}	−0.23
215.598	.600	K	2 500	dc	463 826	4d5	ps63	2.22×10^{10}	−0.81
216.180	.182	K	3		462 577	4d3	ps65	2.29×10^{9}	−1.79
217.394	.395	K	1 500		459 994	4d5	ps65	4.82×10^{10}	−0.47
217.892	.892	K	1 200		458 943	4d3	ps53	5.07×10^{10}	0.44
218.238	.238	K	2 000		458 215	4d3	ps55	5.53×10^{10}	−0.40
218.955	.954	K	5	u	456 715	4d3	8p3	3.11×10^{8}	−2.65
219.063	.062	K	150		456 490	4d3	8p1	7.23×10^{9}	1.28
219.126	.125	K	3		456 358	4d5	ps53	5.09×10^{8}	−2.44
219.391	.391	K	125		455 807	4d3	ps43	2.08×10^{9}	1.82
219.477	.476	K	5		455 629	4d5	ps55	9.39×10^{5}	−5.17
219.847	.846	K	7		454 862	4d3	ps31	2.46×10^{6}	4.75
220.201	.202	K	250		454 131	4d5	8p3	1.09×10^{10}	−1.10
220.642	.641	K	10		453 223	4d5	ps43	8.07×10^{7}	−3.23
221.319	.319	K	1		451 836	4d3	ps45	4.49×10^{7}	3.48
222.592	.593	K	2 000		449 252	4d5	ps45	2.19×10^{10}	−0.79
224.483	.483[1]	K	3 000		445 468	4d5	ps37	6.83×10^{9}	−1.29
226.469	.471	K	3 000		441 562	4d3	ps35	8.66×10^{10}	−0.18
227.801	.804	K	250		438 980	4d5	ps35	1.50×10^{10}	−0.93
228.368	.370	K	450		437 890	4d3	ps33	5.00×10^{9}	1.41
229.262	.266	K	5 000		436 182	4d3	6f5	1.86×10^{11}	0.17
229.677	.680	K	8 000		435 394	4d5	ps27	1.51×10^{11}	0.08
229.723	.726	K	140		435 307	4d5	ps33	3.79×10^{9}	−1.52
230.348	.352	K	2 000		434 126	4d3	ps25	2.43×10^{10}	−0.71
230.433	.437	K	10 000		433 966	4d5	6f7	3.04×10^{11}	0.38
230.628	.633	K	250		433 599	4d5	6f5	2.08×10^{10}	−0.78
230.850	.854	K	200		433 182	4d3	ps23	9.10×10^{9}	1.14
231.728	.731	K	80		431 540	4d5	ps25	2.39×10^{7}	−3.72
232.233	.239	K	2 000		430 602	4d5	ps23	7.27×10^{10}	−0.23
233.113	.117	K	4 000		428 977	4d5	ps17	1.51×10^{10}	0.91
234.187	.192	K	1 500		427 009	4d3	ps21	4.51×10^{10}	−0.43
234.465	.472	K	60		426 503	4d3	ps15	1.13×10^{8}	3.03
235.898	.900	K	2 000		423 912	4d5	ps15	6.71×10^{8}	−2.25
237.719	.716	K	200		420 665	4d3	ps13	1.04×10^{8}	−3.06
239.188	.185	K	1 500		418 081	4d5	ps13	3.01×10^{9}	−1.59
239.409	.411	K	400		417 695	4d3	ps11	1.38×10^{9}	−1.93
240.347	.344	K	50		416 065	4d3	7p3	1.17×10^{10}	1.00
241.050	.047	K	1 500		414 852	4d3	7p1	1.52×10^{10}	−0.88
241.847	.844	K	4 000		413 485	4d5	7p3	4.60×10^{10}	−0.39
241.967	.966	K	50 000		413 279	4d3	d113	1.24×10^{12}	1.04
242.250	.246	K	2 000		412 797	4d3	d115	6.92×10^{10}	−0.22
243.486	.487	K	1 800		410 701	4d5	d113	1.11×10^{11}	−0.01
243.773	.772	K	100 000		410 218	4d5	d115	1.91×10^{12}	1.23
245.155	.153	K	1 500		407 905	4d3	d103	7.74×10^{10}	−0.16
246.717	.713	K	50 000		405 323	4d5	d103	9.07×10^{11}	0.92
248.065	.060	K	25 000		403 120	4d3	d71	4.95×10^{11}	0.66
252.302	.294	K	150 000		396 350	4d5	d97	1.36×10^{12}	1.11

Present Wavelength (Å)	Previous Wavelength (Å)	Ref	Intensity		Wave number (cm^{-1})	Even level	Odd	$gA(s^{-1})$	log(gf)
196.234	.233	K	4		509596	4d3	11p1	1.29E+09	-2.13
197.160	.163	K	5		507202	4d5	11p3	2.16E+09	-1.90
199.828	.835	K	80		500430	4d5	9f7	3.14E+10	-0.73
200.788	.794	K	8		498038	4d3	10p1	1.84E+09	-1.95
201.729	.733	K	15		495715	4d5	10p3	3.14E+09	-1.72
204.619	.620	K	100		488713	4d3	8f5	3.37E+10	-0.68
205.690	.691	K	150		486169	4d5	8f7	5.33E+10	-0.47
207.752	.745	K	8	u	481343	4d3	9p1	2.88E+09	-1.73
208.692	.691	K	60		479175	4d5	9p3	5.04E+09	-1.48
213.018	.017	K	90		469444	4d3	ps75	1.73E+09	-1.93
213.755	.756	K	1,000		467825	4d3	7f5	6.81E+10	-0.33
214.195	.196	K	1,000		466864	4d5	ps75	3.52E+10	-0.62
214.407	.409	K	200		466403	4d3	ps63	5.49E+09	-1.42
214.888	.890	K	1,500		465359	4d5	7f7	1.13E+11	-0.11
214.942	.942	K	110		465242	4d5	7f5	5.88E+09	-1.39

215.598	.600	K	2,500	dc	463826	4d5	ps47	8.51E+10	-0.23
215.598	.600	K	2,500	dc	463826	4d5	ps63	2.22E+10	-0.81
216.180	.182	K	3		462577	4d3	ps65	2.29E+09	-1.79
217.394	.395	K	1,500		459994	4d5	ps65	4.82E+10	-0.47
217.892	.892	K	1,200		458943	4d3	ps53	5.07E+10	-0.44
218.238	.238	K	2,000		458215	4d3	ps55	5.53E+10	-0.40
218.955	.954	K	5	u	456715	4d3	8p3	3.11E+08	-2.65
219.063	.062	K	150		456490	4d3	8p1	7.23E+09	-1.28
219.126	.125	K	3		456358	4d5	ps53	5.09E+08	-2.44
219.391	.391	K	125		455807	4d3	ps43	2.08E+09	-1.82
219.477	.476	K	5		455629	4d5	ps55	9.39E+05	-5.17
219.847	.846	K	7		454862	4d3	ps31	2.46E+06	-4.75
220.201	.202	K	250		454131	4d5	8p3	1.09E+10	-1.10
220.642	.641	K	10		453223	4d5	ps43	8.07E+07	-3.23
221.319	.319	K	1		451836	4d3	ps45	4.49E+07	-3.48
222.592	.593	K	2,000		449252	4d5	ps45	2.19E+10	-0.79
224.483	.483[d]	K	3,000		445468	4d5	ps37	6.83E+09	-1.29
226.469	.471	K	3,000		441562	4d3	ps35	8.66E+10	-0.18
227.801	.804	K	250		438980	4d5	ps35	1.50E+10	-0.93
228.368	.370	K	450		437890	4d3	ps33	5.00E+09	-1.41
229.262	.266	K	5,000		436182	4d3	6f5	1.86E+11	0.17
229.677	.680	K	8,000		435394	4d5	ps27	1.51E+11	0.08
229.723	.726	K	140		435307	4d5	ps33	3.79E+09	-1.52
230.348	.352	K	2,000		434126	4d3	ps25	2.43E+10	-0.71
230.433	.437	K	10,000		433966	4d5	6f7	3.04E+11	0.38

230.628	.633		K	250	433599	4d5	6f5	2.08E+10	-0.78
230.850	.854		K	200	433182	4d3	ps23	9.10E+09	-1.14
231.728	.731		K	80	431540	4d5	ps25	2.39E+07	-3.72
232.233	.239		K	2,000	430602	4d5	ps23	7.27E+10	-0.23
233.113	.117		K	4,000	428977	4d5	ps17	1.51E+10	-0.91
234.187	.192		K	1,500	427009	4d3	ps21	4.51E+10	-0.43
234.465	.472		K	60	426503	4d3	ps15	1.13E+08	-3.03
235.898	.900		K	2,000	423912	4d5	ps15	6.71E+08	-2.25
237.719	.716		K	200	420665	4d3	ps13	1.04E+08	-3.06
239.188	.185		K	1,500	418081	4d5	ps13	3.01E+09	-1.59
239.409	.411		K	400	417695	4d3	ps11	1.38E+09	-1.93
240.347	.344		K	50	416065	4d3	7p3	1.17E+10	-1.00
241.050	.047		K	1,500	414852	4d3	7p1	1.52E+10	-0.88
241.847	.844		K	4,000	413485	4d5	7p3	4.60E+10	-0.39
241.967	.966		K	50,000	413279	4d3	d113	1.24E+12	1.04
242.250	.246		K	2,000	412797	4d3	d115	6.92E+10	-0.22
243.486	.487		K	1,800	410701	4d5	d113	1.11E+11	-0.01
243.773	.772		K	100,000	410218	4d5	d115	1.91E+12	1.23
245.155	.153		K	1,500	407905	4d3	d103	7.74E+10	-0.16
246.717	.713		K	50,000	405323	4d5	d103	9.07E+11	0.92
248.065	.060		K	25,000	403120	4d3	d71	4.95E+11	0.66
252.302	.294	.3034	K	150,000	396350	4d5	d97	1.36E+12	1.11
253.779	.770	.7778	K	125,000	394044	4d3	d105	9.17E+11	0.95
255.443	.443		K	400	391477	4d5	d105	1.48E+10	-0.84
264.148	.151		K	250	378576	5s1	10p3	3.86E+09	-1.39
273.508	.511		K	100,000	365620	4d5	5f7	1.90E+11	0.33
273.894	.898		K	100,000	365105	4d3	5f5	2.53E+11	0.45
275.847	.851		K	150	362520	4d5	5f5	4.72E+09	-1.27

THEORETICAL CALCULATIONS

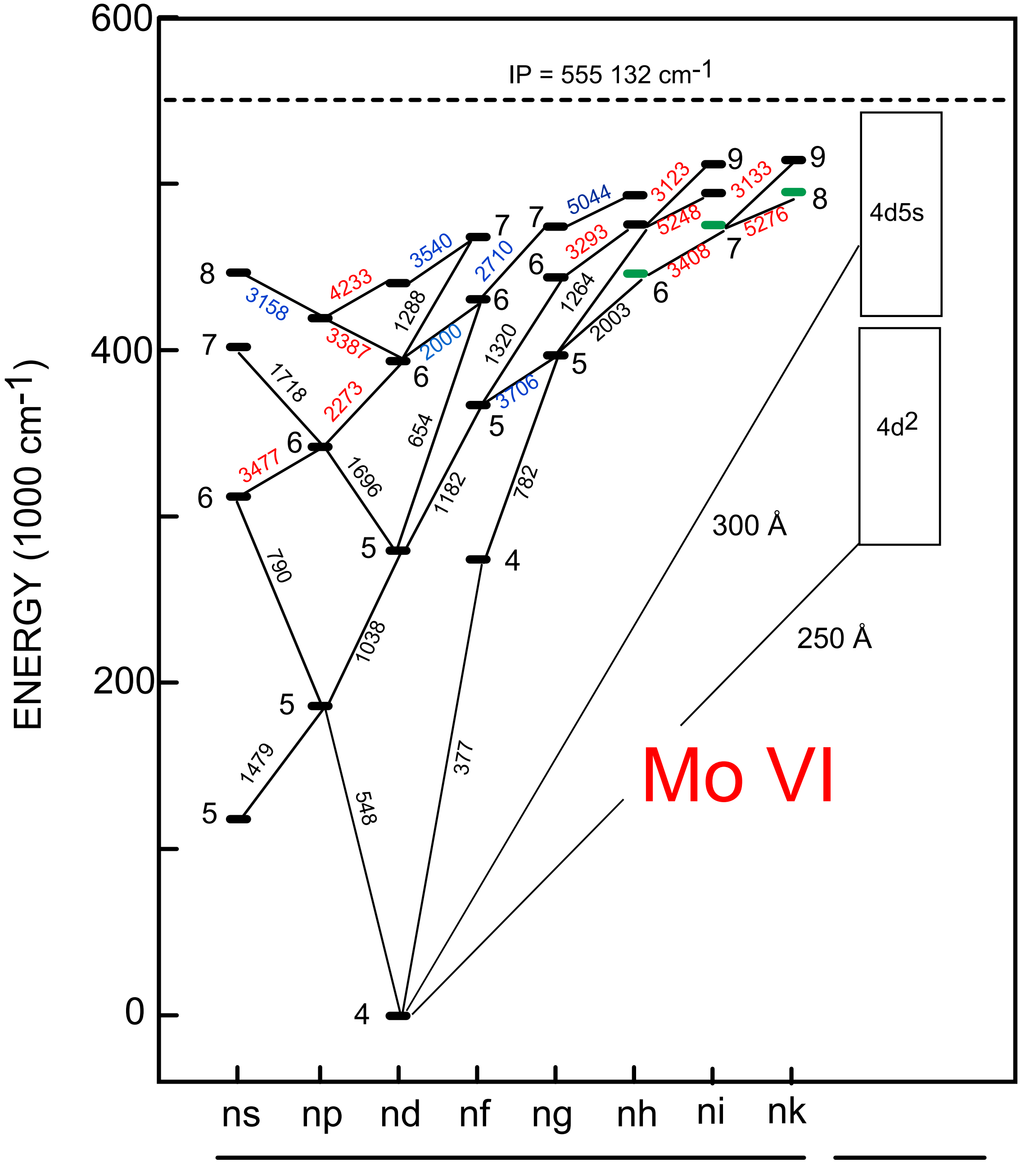
- Cowan codes: Hartree-Fock; Diagonalization; Least-Squares Fit (RCN; RCG; RCE)

- SIMILAR TO KANCEREVICIUS ET AL.

- RELATIVISTIC MODE (not important)

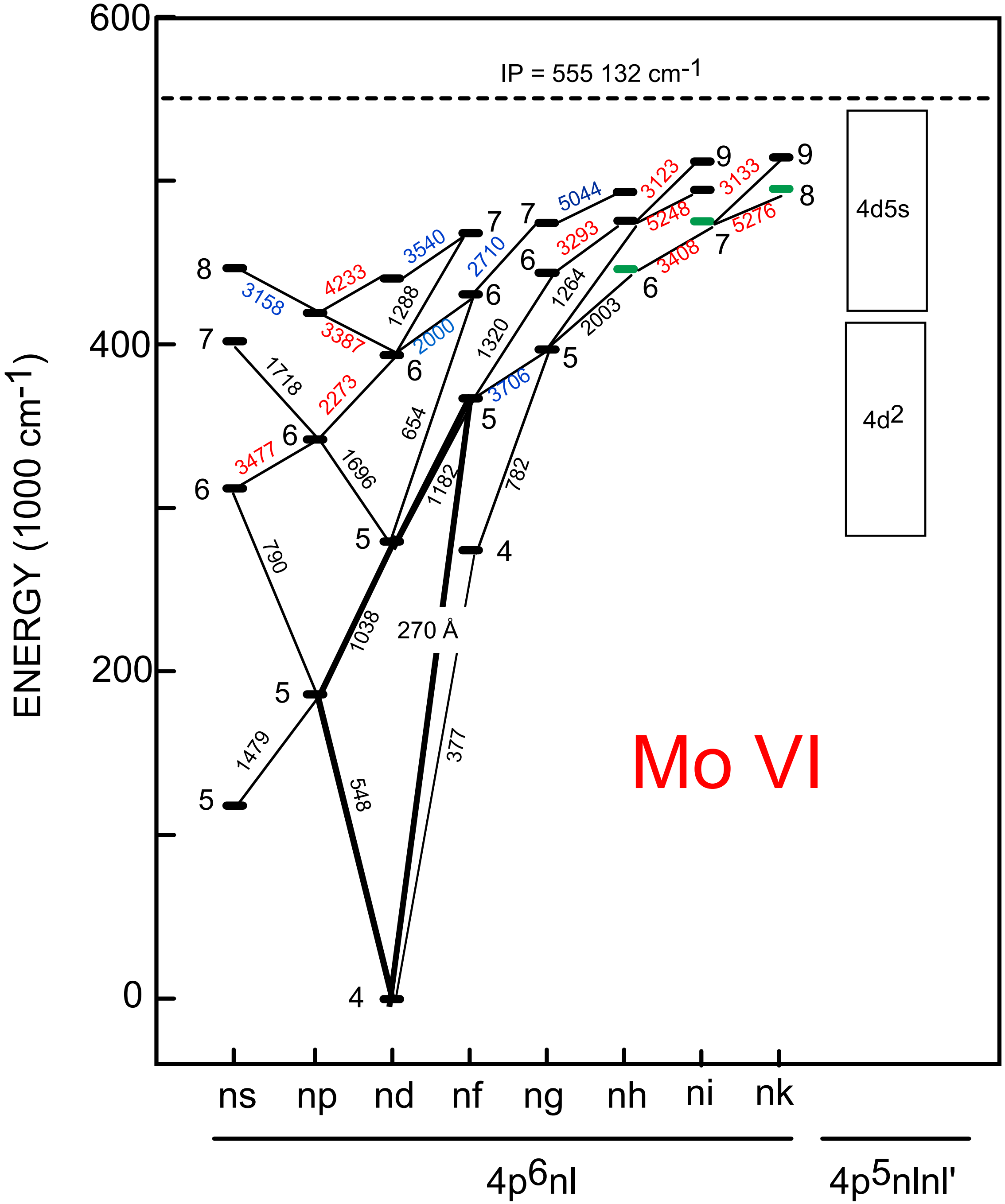
- LARGE MIXTURES: 4f, 5f, 6f, 6p, 7p, 8p with $4p^5 4d^2$ and $4p^5 4d5s$

- MAIN USE: SELECT LONG WAVELENGTH CI LINES FOR LEVEL OPTIMIZATION - 24 LINES



Penning discharge
Used for ionization energy
New lines

SCHEMES FOR ACCURATE RITZ-TYPE WAVELENGTHS



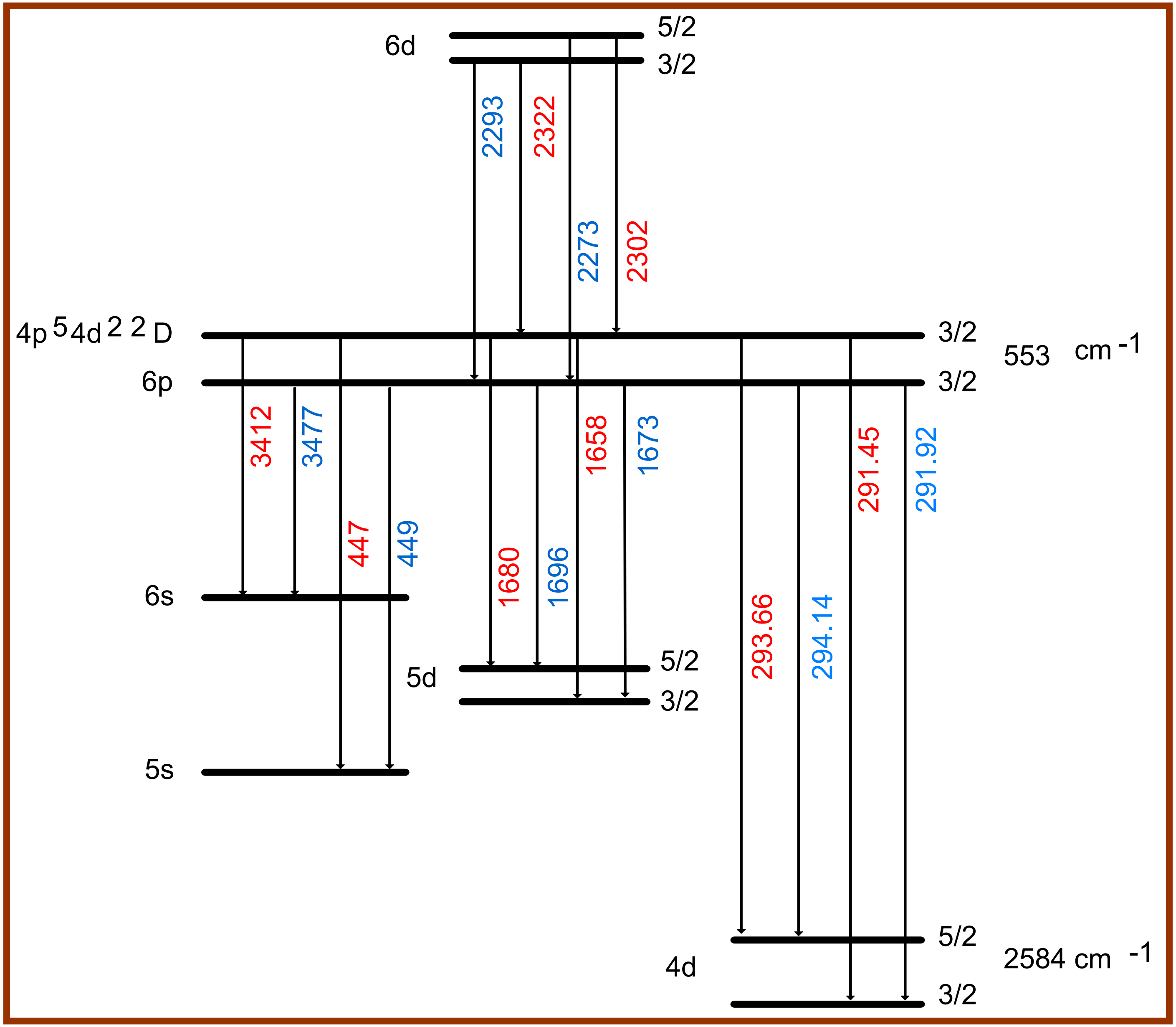
RITZ SCHEME #1

only allowed lines

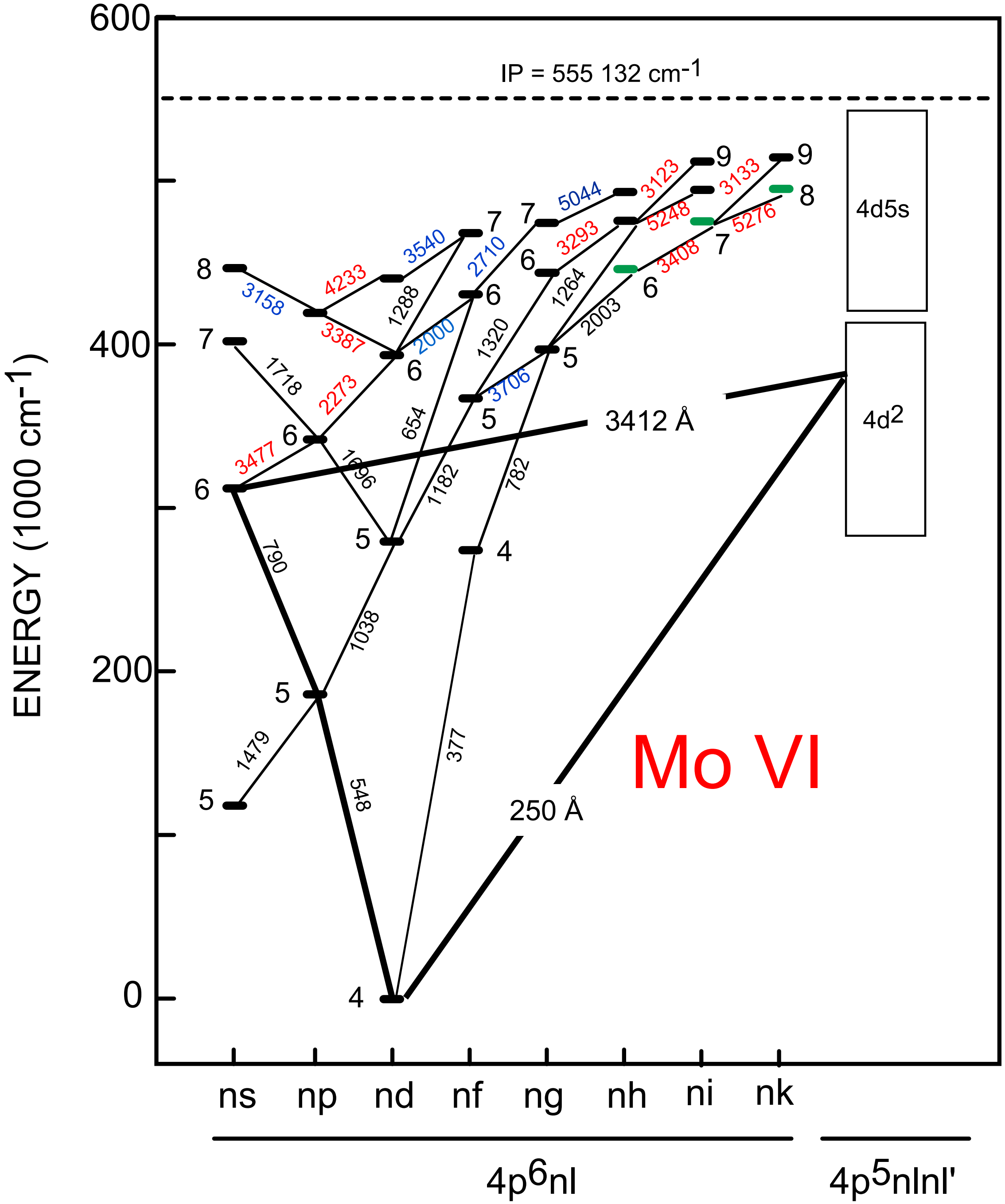
Penning discharge

Used for ionization energy

New lines



CONFIGURATION INTERACTION



RITZ SCHEME #2 uses CI lines

Penning discharge

Used for ionization energy

New lines

Wavelengths (Å) of selected lines of Mo VI as calculated from optimized level values.

Even level	Odd level	Observed wavelength	Intensity[a]		Calculated wavelength	Uncertainty
4d3	7f5	213.755	1,000		213.7530	0.0004
4d5	7f7	214.888	1,500		214.8870	0.0004
4d5	7f5	214.942	110		214.9399	0.0004
4d3	8p3	218.955	5	u	218.9533	0.0004
4d3	8p1	219.063	150		219.0605	0.0008
4d5	8p3	220.201	250		220.1989	0.0004
4d3	6f5	229.262	5,000		229.2624	0.0005
4d5	6f7	230.433	10,000		230.4334	0.0005
4d5	6f5	230.628	250		230.6284	0.0005
4d3	7p3	240.347	50		240.3450	0.0005
4d3	7p1	241.050	1,500		241.0488	0.0005
4d5	d97	252.302	150,000		252.3034	0.0006
4d3	d105	253.779	125,000		253.7778	0.0006
4d5	d105	255.443 255.443 K	400		255.4527	0.0006

4d5	5f7	273.508	100,000		273.5083	0.0007
4d3	5f5	273.894	100,000		273.8950	0.0006
4d5	5f5	275.847	150		275.8469	0.0007
4d3	d95	286.299	25,000		286.3000	0.0007
4d3	d83	288.278	80		288.2768	0.0011
4d5	d87	288.920	10,000		288.9182	0.0008
4d5	d83	290.439	4,000		290.4399	0.0012
4d3	d73	291.446	250		291.4479	0.0007
4d3	6p3	291.916	15		291.9176	0.0007
4d3	6p1	293.625	2,500		293.6247	0.0007
4d5	d73	293.660	6,000		293.6590	0.0008
4d5	6p3	294.137	1,000		294.1359	0.0008
4d3	d85	296.673	25,000	p	296.6734	0.0008
4d5	d85	298.963	4,000		298.9648	0.0008
4d5	d57	314.956	120,000		314.9562	0.0009
4d3	d55	317.302	40,000		317.3037	0.0009

4d5	d47	318.578	20,000		318.5798	0.0009
4d5	d55	319.926	4,000		319.9263	0.0009
4d5	d37	323.092	8,000		323.0946	0.0009
5s1	7p3	337.446	80		337.4468	0.0003
5s1	7p1	338.834	30		338.8358	0.0003
4d3	4f5	374.465	300,000		374.4656	0.0012
4d5	4f7	377.540	400,000		377.5389	0.0013
4d5	4f5	378.124	8,000		378.1237	0.0013
5s1	6p3	448.757	100		448.7589	0.0005
5s1	6p1	452.804	60		452.8059	0.0005
7s1	5p1	457.966	40		457.9654	0.0007
7s1	5p3	468.536	80		468.5368	0.0006
6d5	5p3	501.954	7		501.9552	0.0006
5d3	7f5	540.546	10	p	540.5283	0.0003
5d5	7f7	542.496	20		542.4951	0.0003
5d5	7f5	542.826	3		542.8326	0.0003
6g7	4f5	565.322	200,000		565.3220	0.0004
6g9	4f7	566.621	250,000		566.6231	0.0005

5d3	6f5	652.072	50,000		652.0779	0.0005
5d5	6f7	653.857	40,000		653.8624	0.0006
5d5	7p3	754.957	25,000		754.9583	0.0004
5d3	7p1	757.413	15,000		757.4138	0.0006
6s1	5p1	761.016	800,000		761.0214	0.0016
5g7	4f5	780.432	700,000		780.4323	0.0009
5g9	4f7	782.918	800,000		782.9169	0.0011
6s1	5p3	790.660	1,600,000		790.6662	0.0016
7g9	5f7	950.263	100,000	w	950.2641	0.0018
8s1	6p3	950.855	30,000		950.8616	0.0009
7d3	6p1	1011.184	4,000		1011.1799	0.0011
7d5	6p3	1029.565	2,000		1029.5603	0.0009
5d5	5f7	1182.143	1,000,000		1182.1418	0.0018
5d3	5f5	1215.397	800,000		1215.3940	0.0014
6d3	7f5	1224.529	150		1224.5270	0.0014
5d5	5f5	1227.102	8,000		1227.1068	0.0012
6d5	7f7	1228.620	400	w	1228.6182	0.0013
6g7	5f5	1268.495	3,000		1268.4862	0.0013

IONIZATION ENERGY

TRAWICK (1934)	543 600 cm^{-1}
KIESS (1956); AEL (Zr IV series)	549 000 cm^{-1}
EDLÉN et al. (1985)	555 132 ± 2 (?) cm^{-1}

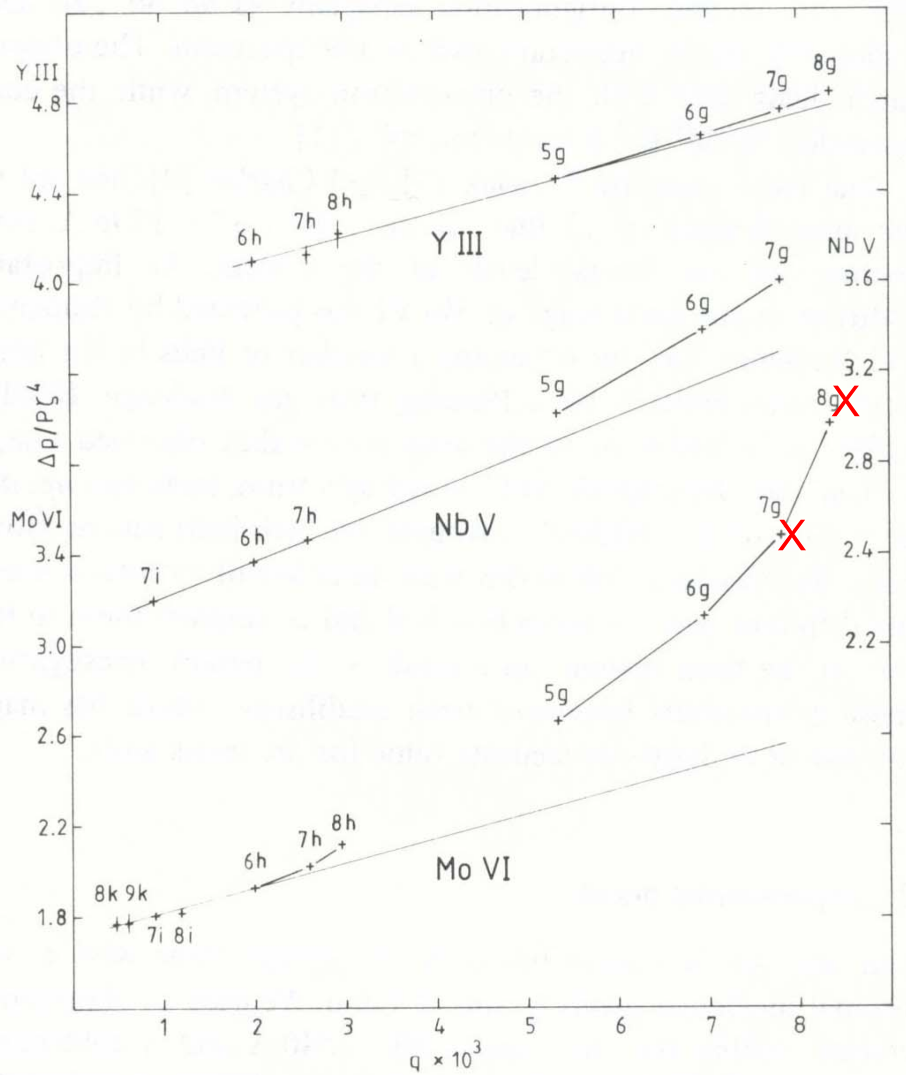
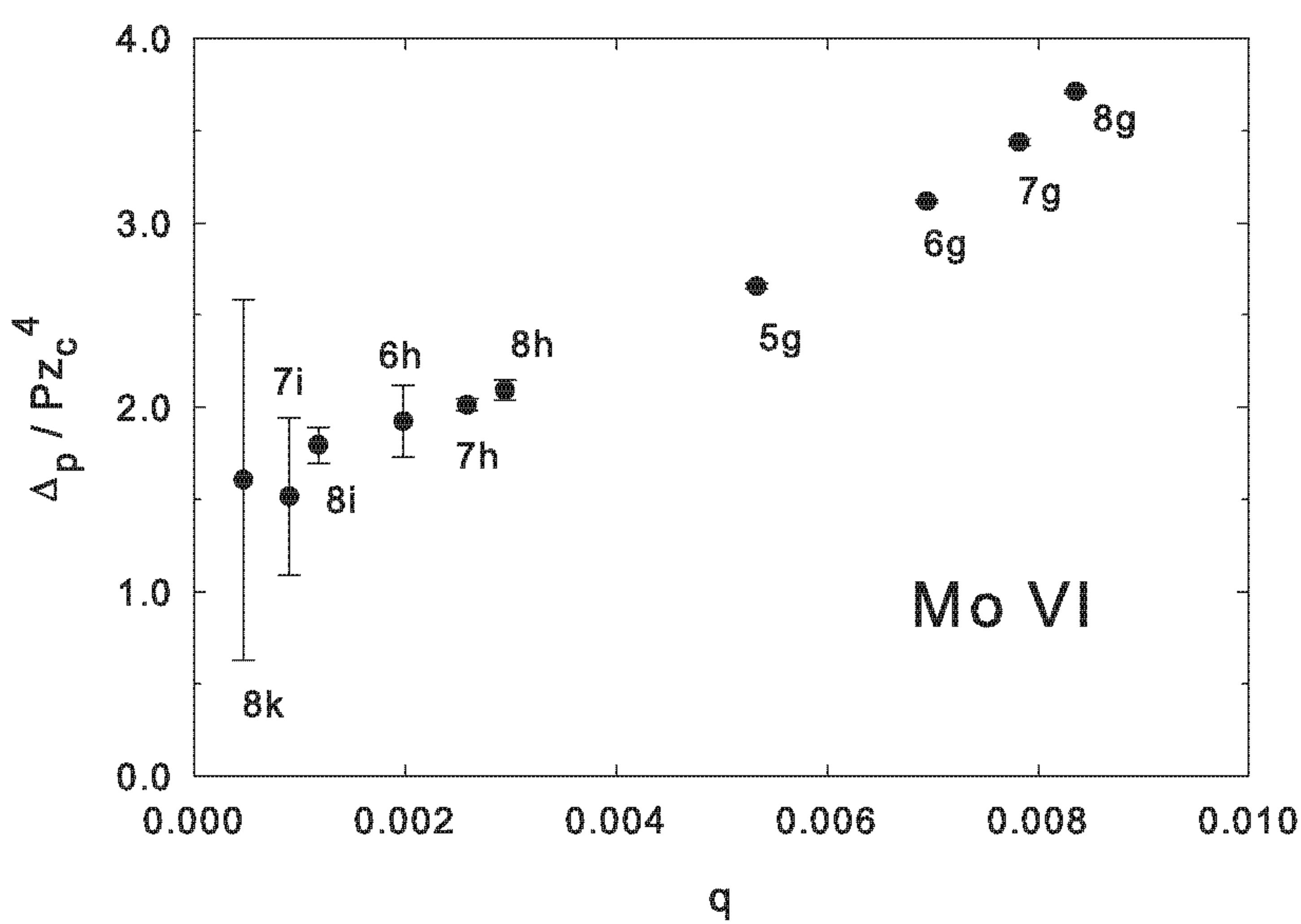


Fig. 4. Comparison of polarization diagrams for YIII, Nb V and Mo VI, normalized by the factor ζ^{-4} ($\zeta = Z - 36$). The anomalous behaviour of the ng series is explained by interaction with the ^2G term of $4s4p^6 4d^2$.

“The anomalous behaviour of the ng series is explained by interaction with the ^{2}G term of $4s4d^6 4d^2$.”


4.0
3.0
2.0
1.0
0.0
0.000
0.002
0.004
0.006
0.008
0.010
q
Δ_p / Pz_c^4
8g
7g
6g
5g
8h
6h
7h
7i
8i
8k
Mo VI

$\Delta_p = T - T_{hydrogenic}$

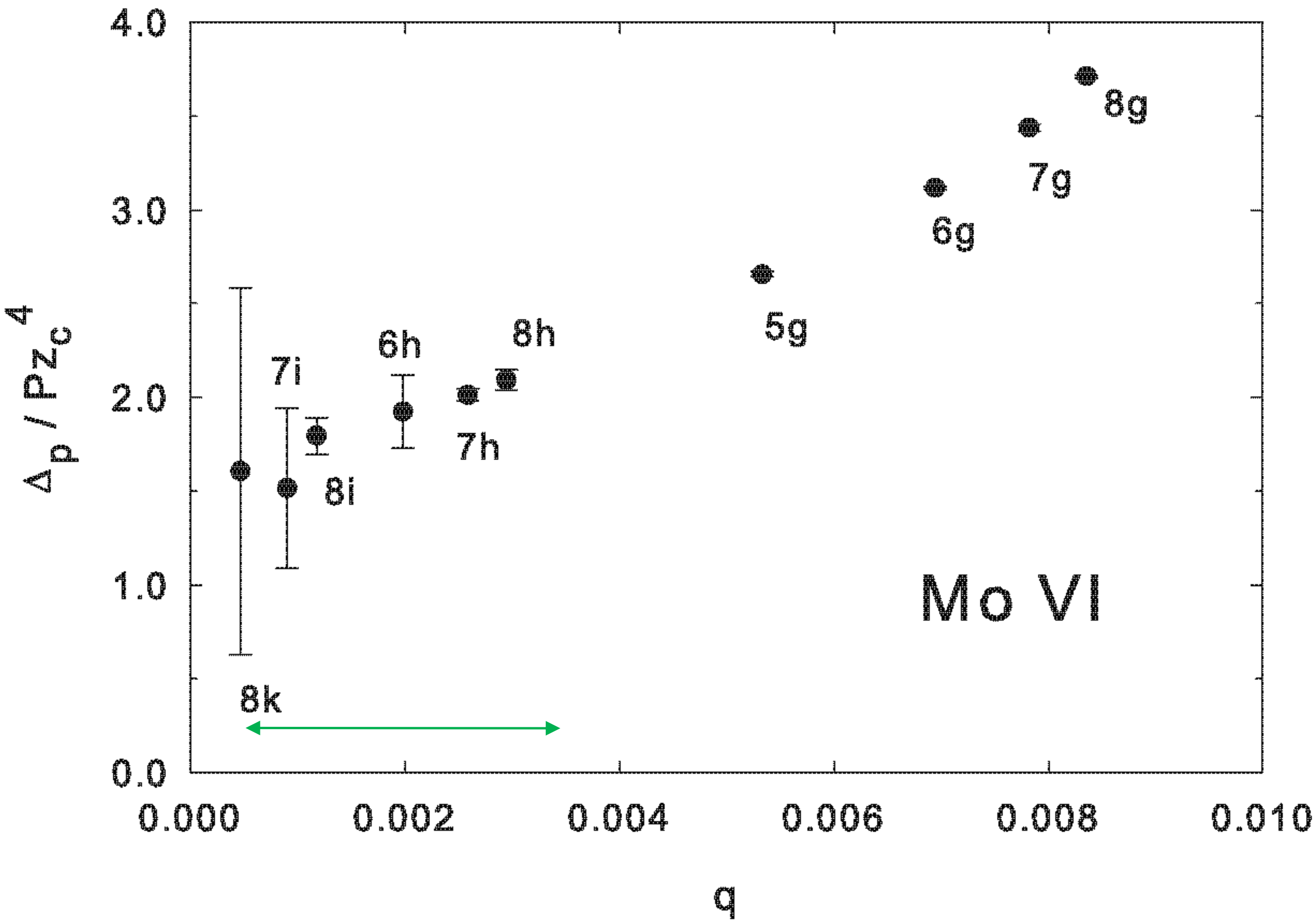
$\Delta_p = \alpha_d\, R \langle r^{-4} \rangle + \alpha_q\, R \langle r^{-6} \rangle$

$\alpha_d =$ dipole polarizability

$\alpha_q =$ quadrupole polarizability

$P = R \langle r^{-4} \rangle / Z_c^{\,2}$

$q = \langle r^{-6} \rangle / Z_c^{-6} \times Z_c^{\,4} / \langle r^{-4} \rangle$



(ng levels not perturbed by $4s4p^24d^2$)

Values for the ionization energy (cm^{-1}) of Mo VI determined from various levels.

Levels	Method	Limit	Unc.
5s-8s	Quadratic quantum defect	555100.4	
5g-8g	Quadratic quantum defect	555031.8	
5g-8g	Polarization formula	555022.7	2.3
6h-8h	Linear quantum defect	555114.6	
6h-8h	Polarization formula	555115.6	
6h-8h, 7i-8i,8k	Polarization formula	555127.5	0.8
6h, 7i, 8k	Polarization formula	555129.7	
	Edlén et al.	555132.0	2 (?)
5g, 6h, 7i, 8k	Polarization formula	555125.7	2.3

IONIZATION ENERGY

TRAWICK (1934)	543 600 cm^{-1}
KIESS (1956); AEL (Zr IV series)	549 000 cm^{-1}
EDLÉN et al. (1985)	555 132 ± 2 cm^{-1}
READER (2010)	555 127.5 ±1.7 cm^{-1}

Lund, sept. 5, 1998

Dear Larry,

Your letter of july 29 made me very happy. How much more would it have enjoyed Bengt, if he were alive!

I am grateful to you for having taken the trouble to inform me about Joe Reader's talk at Santa Fé which confirmed that Bengt's levels to determine the ionization potentials of MO VI were confirmed to be correct. - Indeed Bengt felt unhappy to have allowed Chaghtai to use his name as coauthor. I am sure Bengt would have been more careful to read Chaghtai's manuscript if he had been in better health. He was just recovering from his first stroke at that time.

My very best wishes for your health and continual work

Fond regards,

Friedel Edlén

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Fond regards,

Friedel Edl'en

ROMANOV & STRIGANOV'S LINES OF Mo VI

RS	RS	RS	JR	Edlén
6336.04	5	4f-5d	4f-5d	
6328.11	1.5			
6198.21	1.4			
6195.84	1.8			
6189.16	1.8			
6188.67	11	4f-5d	4f-5d	
6166.09	1.6			
6035.62	0.75	4f-5d	4f-5d	
5871.37	1.5		7d-8p	
5619.63	1.7		8d-8f	
5585.08	1.0		8d-8f	
5448.82	7.5			5f-6d
5355.81	2.5			
5276.86	45	7i-8k	7i-8k	
5247.45	35	7h-8i	7h-8i	
5043.55	10	7g-8h	not obs	
5042.77	8.5	7g-8h	not obs	
4501.73	1		not obs	
4495.55	9		not obs	
4490.73	11		not obs	
4272.95	8	7p-7d	7p-7d	

RS	RS	RS	JR	Edlén
4232.04	100	7p-7d	7p-7d	
4062.04	60	7p-7d	7p-7d	
4054.55	3		7f-8g	
3735.32	90	6s-6p	6s-6p	
3538.39	20		7d-7f	
3510.27	6.6		5d-4d^2	
3484.77	13	6d-7p	6d-7p	
3476.60	200	6s-6p	6s-6p	
3411.11	25		6s-4d^2	
3408.60	200	6h-7i	6h-7i	
3386.98	20	6d-7p	6d-7p	
3343.20	1.5	6d-7p	6d-7p	
3323.75	22		5f-5g	5f-5g
3293.29	50	6g-7h	6g-7h	
3293.00	45	6g-7h	6g-7h	
3133.32	10	6f-7g	not obs	7i-9k
3122.43	10	6f-7g	not obs	7h-9i
2301.48	30		6d-4d^2	
2292.73	15	6p-6d	6p-6d	
2272.58	200	6p-6d	6p-6d	
2192.57	100	6p-6d	6p-6d	

Mushtaq, Chaghtai, Rahimullah (1979)

4 of 19 levels of $4p^5 4d5s$ confirmed by Kancerevicius et al. (1991)

Tauheed, Rahimullah, Chaghtai (1985)

5 of 38 levels of $4p^5 4d^2$ confirmed by Kancerevicius et al. (1991)

1 of 35 $4p^6 nl$- $4p^5 4d^2$ 2-electron jump CI lines confirmed by Reader (2010)

Edlén, Tauheed, Rahimullah, Chaghtai (1985)

- 8p and 6f levels rejected by Kancerevicius et al. (1991)

- 8d, 7g, 8g levels rejected by Reader (2010)

- Ionization energy - ~ not affected

Kancerevicius, Ramonas, Ryabtsev, Churilov (1991)

- 9 lines of 120 not Mo VI - (V, VII, VIII-only 2 spark regimes?): 5 levels dropped

- 2 new levels of $4p^54d^2$

- $4p^54d(^1P)5s\ ^2P_{1/2,\ 3/2}$ levels still unknown (should be strong to $4p^55s$)

- New least-squares fit; rms error 161 cm-1 vs 281 cm-1 (dropped bad levels)

- Similar admixtures $4p^54d^2$ and $4p^54d5s$ – 4f, 5f, 6f, 6p, 7p, 8p

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Mo VI $J = 3/2, 5/2$ energy levels, oscillator strengths and Landé g-values

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Abstract
Relativistic configuration interaction calculations have been performed for Mo VI $4p^5\,4d^2$ $J = 5/2$ and $nf\,^2F_{5/2}$ ($n = 4$–6) wavefunctions. Level energies and E1 oscillator strengths for transitions between these states and the $nd\,^2D$ ($n = 4$–6) states have been obtained. The calculated LS compositions of all 11 levels of $4p^5\,4d^2$ $J = 5/2$ have been found to be in good agreement with other designations. While most calculated level energies agree well with the most recent experimental work, large discrepancies in a few (upper) levels do exist. The oscillator strength of all 84 transitions are computed, and 36 of the largest ($f > 0.001$) are presented here. Most of the oscillator strengths are computed for the first time.

PACS numbers: 31.25.Jf, 32.70.Cs

1. Introduction

Mo VI is a member of the Rb I isoelectronic sequence with $4p^6\,4d$ as its ground-state configuration. It is important for diagnostics of controlled fusion plasmas.

Our interest in this species came about from our work on Mo V [1], where we calculated the positions of the $4p^5\,4d^3$ levels. These levels were interpenetrating the $4d(np + 4f)$, 5s5p levels. The changing core ($4p^5$ vs $4p^6$) population means fewer correlation effects nearly cancel, thus requiring the use of much more extensive wavefunctions. It was suggested [2] that Mo VI might offer a test of our methods, as it was simpler (fewer electrons) and that some results were available for the $4p^5\,4d^2$ levels.

The investigation of Mo VI began in the early 1930s. So far, the one-electron spectra of Mo VI have been extensively studied, but study of the core-excited states such as the $4p^5\,4d^2$ and $4p^5\,4d\,5s$ states have gained much less attention. It's been established that the $4p^5\,4d^2$ states are strong perturbers of the nf and np one-electron spectra, and they are responsible for an important part of Mo VI's spectrum. However, identifying them experimentally is not an easy task. For example, identification of the $4p^6\,4d$–$4p^5\,4d^2$ transitions is complicated by three facts [3]. Firstly, there are other transitions in Mo VI that lie in the same spectral region. Secondly, there are transitions in Mo V that behave very similarly to the transitions of interest. Finally, there is strong interaction between the $4p^6\,nf$ states and the $4p^5\,4d^2$ states. In 1985, Tauheed *et al* [4] measured the energy values of $4p^5\,4d^2$ for the first time and established 38 out of the total 45 levels. In 1991, Kancerevicius *et al* [3] published their results for Mo VI, giving energy values of 37 out of 45 levels of $4p^5\,4d^2$ (some of them are available on the NIST database [5]) and 20 out of 23 levels of $4p^5\,4d\,5s$. For the $J = 5/2$ levels of $4p^5\,4d^2$, the differences between Tauheed *et al* and Kancerevicius *et al* are sometimes large, varying from 0 to 6300 cm^{-1} and are not in one direction.

The strong interaction between $4p^6\,nf$ and $4p^5\,4d^2$ also complicates the computations for their level energies. Before this work, there was only one semi-empirical computation by Cowan for these levels. The results were not formally published, but they can be derived from [4]. Comparing with [3], his calculated levels are too high by 972 to 7772 cm^{-1}.

These large discrepancies, while illustrating the elusiveness of the $4p^5\,4d^2$ levels, provided motivations to the present calculation and one on-going experiment work [2]. In our work, we have performed relativistic configuration interaction (RCI) calculations for energy values of Mo VI $4p^6\,nd$ ($n = 4$–6) even parity states, $4p^6\,nf$ ($n = 4$–6) and $4p^5\,4d^2$ $J = 5/2$ odd parity states, and oscillator strengths of transitions between them. To simplify notations, we will drop the closed core in the one-electron configurations from now on. We will also use 'Rn' to denote the levels of $4p^5\,4d^2$ with the lowest one being R1.

Mo VI J=3/2, 5/2 ENERGY LEVELS , OSCILLATOR STRENGTHS, AND LANDE g-VALUES

Lin Pan and Donald R. Beck; Physica Scripta (2006)

- Relativistic configuration interaction calculation
- Relativistic screened hydrogenic wave functions
- Correlations: 300 configurations in core
- Final matrix: 19621x19621
- “Virtual subshells”

Comparison of *f*-values of Pan and Beck (2006) with present values.

Transition		Wavelength[a]	Note[b]	Pan and Beck Coulomb	Pan and Beck Babushkin	*f*(present)	Intensity
4d3	4f5	374.465		0.2849	0.2896	0.3226	300,000
	d35	329.827		0.0087	0.0090	0.0090	30,000
	d55	317.302		0.0628	0.0666	0.0695	40,000
	d65	313.944		0.0143	0.0155	0.0270	30,000
	d75	303.147		0.0023	0.0025	0.0044	1,500
	d85	296.673		0.0771	0.0808	0.0766	25,000
	d95	286.299		0.0207	0.0221	0.0212	25,000
	5f5	273.894		0.4451	0.4835	0.7099	100,000
	d105	253.779		1.7480	1.8422	2.2140	125,000
	d115	242.250		0.1346	0.1404	0.1523	2,000
	6f5	229.262		0.2863	0.3061	0.3672	5,000
5d3	d75	2125.495	b	0.0011	0.0014	0.0023	
	d85	1843.481		0.0417	0.0551	0.0432	25,000
	d95	1504.694		0.0115	0.0140	0.0104	8,000
	5f5	1215.397		0.6207	0.7048	0.7858	800,000
	d105	899.123		0.2545	0.2365	0.2598	300,000
	6f5	652.072		0.1502	0.1804	0.1702	50,000
6d3	d95	2711.377	b	0.0041	0.0056	0.0028	
	5f5	4747.849		0.2091	0.2781	0.2399	8,000
	d105	12690.645	b	0.2282	0.1853	0.2000	
	d115	3754.688	b	0.0055	0.0041	0.0048	
	6f5	1999.366		0.9901	1.0228	1.0002	25,000
4d5	4f5	378.124		0.0136	0.0139	0.0153	8,000
	d55	319.926		0.0082	0.0090	0.0103	4,000
	d75	305.539		0.0101	0.0109	0.0159	20,000
	d85	298.963		0.0146	0.0154	0.0158	4,000
	5f5	275.847		0.0056	0.0062	0.0090	150
	d105	255.443		0.0256	0.0269	0.0242	400
	d115	243.773		2.1563	2.2486	2.8350	100,000
	6f5	230.628		0.0250	0.0268	0.0277	250

THANK YOU

END OF STORY