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ID	Doc Type	Document Description	No of Pages	Doc Date	Restrictions
171900	MEMO	R. KIMMITT TO C. HILL RE RENEWAL OF MEMORANDUM OF COOPERATION	1	1/26/1984	B1
171901	MEMO	J. MATLOCK TO MCFARLANE RE RENEWAL OF MEMORANDUM OF COOPERATION	1	1/23/1984	B1
171902	MEMO	C. HILL TO MCFARLANE RE RENEWAL OF MEMORANDUM OF COOPERATION	3	1/5/1984	B1
171903	REPORT	RE EXTENSION OF MEMORANDUM OF COOPERATION	3	ND	B1
171904	MEMO	COPY OF DOC #171900 (R. KIMMITT TO C. HILL RE RENEWAL OF MEMORANDUM OF COOPERATION)	1	1/26/1984	B1

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TO MCFARLANE FROM HILL, C DOCDATE 05 JAN 84

KEYWORDS USSR TECHNOLOGY TRANSFERS

SUBJECT: RENEWAL OF MEMORANDUM OF COOPERATION BETWEEN US NATL BUREAU OF OF STANDARDS & ACADEMY OF SCIENCES USSR

ACTION: PREPARE MEMO FOR MCFARLANE DUE. 09 JAN 84 STATUS S FILES

FOR ACTION	FOR CONCURRENCE		FOR INFO
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C	1/31	RMK ggd		JM, JF, JL, Index

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National Security Council
The White House

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Bob Kimmitt	2	K	
John Poindexter	4		
Wilma Hall	5		
Bud McFarlane	6	M	A
Bob Kimmitt			
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Situation Room			
Rosie	3		Correction Tab II

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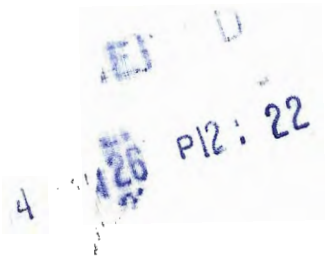
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Bob Kimmitt			
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Rosie	3	done	Correction Tab II

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171902	MEMO C. HILL TO MCFARLANE RE RENEWAL OF MEMORANDUM OF COOPERATION	3	1/5/1984	B1

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171903	REPORT RE EXTENSION OF MEMORANDUM OF COOPERATION	3	ND	B1

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UNITED STATES DEPARTMENT OF COMMERCE
National Bureau of Standards
Washington, D.C. 20234

2/12

NOV 16 1983

MEMORANDUM FOR Byron Morton
Deputy Director, EUR/SOV
Department of State

From: Edward L. Brady Edward L. Brady
Associate Director for
International Affairs

SUMMARY: The National Bureau of Standards recommends that, subject to overriding foreign policy objections, it be authorized to propose to the USSR Academy of Sciences that the current Memorandum on Cooperation (MoC) between the two institutions, now scheduled to terminate December 12, 1983, be renewed for an additional five-year period. NBS officials have critically reviewed the implementation of the MoC and have concluded that NBS has acquired technical information on work in progress in institutes of the Academy of Sciences that would be difficult, if not impossible, to obtain by other means. This information has been of significant benefit to the accomplishment of NBS scientific objectives. END SUMMARY

Background: The NBS/ASUSSR Memorandum on Cooperation, a copy of which is attached as Attachment A, derives from extended negotiations dating back to a proposal originally made in 1974 by the late President of the USSR Academy of Sciences, M. V. Keldysh. It was signed at Moscow by Academy Vice President Ye. P. Velikhov and NBS Director Ernest Ambler on December 13, 1978, with a period of validity of five years. It has the status of an implementing protocol of the intergovernmental Agreement on Cooperation in the Fields of Science and Technology, dated May 24, 1972. Despite the non-renewal, on foreign policy grounds, of this umbrella Agreement upon its termination in 1982, it was determined by a committee representing the Department of State and other agencies of the Executive Branch that activities under the MoC should continue because NBS acquisition of information under the program was considered beneficial to U.S. interests. The possibility of such continuation was allowed for in Paragraph 2 of Article 8 of the umbrella Agreement which states that "The termination of this Agreement shall not affect the validity of agreements made hereunder between agencies, organizations and enterprises of both countries." This, then, is the legal basis under which implementation of the MoC has continued to the present time.

History of Implementation of the MoC: During the past five years, the MoC has provided NBS with an operating flexibility and broad technical

scope hitherto unavailable in our interactions with leading institutions and scientists of the USSR and has effectively served to promote the acquisition of unpublished information from USSR research institutions and the achievement of mutually desired scientific objectives, through joint work in their own laboratories as well as in ours. Each side has appointed its own Coordinating Council to evaluate, monitor, and guide the joint activities and scientific progress under the MoC. The high-level significance that the Soviet side attaches to the MoC is demonstrated by the composition of its Coordinating Council, comprised of Academician Yu. A. Osip'yan, Director of the USSR Institute for Solid State Physics, as Chairman, plus eight other renowned Soviet scientists, many of whom are directors of leading research institutes and have Academy rank. The NBS Coordinating Council consists of the NBS Director, Ernest Ambler, as Chairman, plus senior members of the NBS staff.

As written, the MoC permits a broad program of scientific cooperation between NBS and research institutes of the ASUSSR and specifically mentions the fields of thermal physics and thermodynamics, materials science, spectroscopy, chemistry and chemical kinetics, and cryogenic science. However, other fields of science may be included by mutual agreement. Although the MoC provides for an annual quota of up to 14 man-months of long-term visits (2-6 months) by each side to the other, plus a quota of up to 6 man-months of short-term visits by senior scientists and program managers, we have not yet approached these upper limits in our cooperative activities. Rather, the program has progressed on a more modest and selective scale at an annual cost to NBS of about $8-12K for transportation and subsistence. The Soviet side has preferred visits of longer duration (up to 3 months), whereas NBS scientists have concentrated on shorter visits (2 weeks to 1 month). The overall usage of the quota has been in favor of the Soviets by a ratio of about 2 Soviet visitors to 1 NBS, but the technical benefits are judged to have been generally equal.

NBS scientists who have participated in the program have without exception reported that Soviet willingness to cooperate at the working scientist level in an effort to make activities scientifically valid and productive is quite high. For example, NBS scientist Dr. Daniel Kelleher, who returned just last month from a two-week familiarization visit to Soviet laboratories, has reported that he encountered a number of forefront Soviet scientific programs that had not previously been known to him and that he had identified several areas where a joint effort would probably lead to significant, mutual scientific payoff. He further commented that non-renewal of the MoC would cut off a source of useful information for him. This observation is in accord with the general view of NBS that the full potential of benefit from the MoC has not yet been exploited.

This is not to say, however, that the program runs entirely smoothly. Bureaucratic and logistical problems on the Soviet side continue to interfere with gaining the maximum possible benefit from the cooperation. The recent one-month visit of NBS scientist Dr. J. Reader in the USSR is an example. Although considered by us to be a technical success, it nevertheless did not succeed in achieving the full benefits that were expected because of failure on the Soviet side to provide already agreed-upon arrangements and laboratory visits. NBS has sent a message of protest to the Soviets in which we request an explanation of this case before we proceed with processing of the applications of three Soviet scientists who have applied to visit NBS under the MoC.

At present, five applications for exchange visits are pending under the MoC--three from the Soviet side (involving three scientists), and two from the NBS side (involving six scientists). The Soviet proposals are in the fields of atomic and molecular spectroscopy, and the NBS proposals are in the fields of chemical thermodynamics and measurement methodology for non-ionizing electromagnetic radiation. We anticipate significant scientific benefit from both of the U.S. proposals, but we are particularly interested in the last-mentioned because of the wide difference between current U.S. and USSR exposure standards in this area.

Assessment of Scientific and Technical Benefits and Their Balance: All NBS participants say that the scientific benefit to their own programs has been significant. One NBS scientist has said that only by visiting and asking questions could he have learned all the details of the experimental techniques used by Soviet scientists in his field. Such details are ordinarily not published, or if they are published, they appear in USSR journals or reports that are difficult to obtain and difficult to read because of the language barrier. The NBS program of collaboration with the USSR in the compilation and evaluation of quantitative data on the physical and chemical properties of matter, which started several years before the establishment of the umbrella agreement for cooperation, has given NBS the benefit of several dozen man-years of high-quality scientific output. Similar benefits are characteristic of all of the cooperative interactions between NBS and USSR laboratories.

As a tangible product of the cooperation, joint publications in the archival technical literature have appeared or are in preparation in the fields of thermodynamic data analysis, crystal structure, molecular spectroscopy, and atomic spectroscopy. Several reprints of joint publications in the latter area are attached as Attachment B. These illustrate the contributions that joint research can make to NBS priority programs, in this case, the provision of data useful for diagnostic work in the DOE fusion energy efforts.

In some cases, the scale of benefits is decidedly tipped in favor of NBS. For example, NBS scientist Dr. K. Evenson reported that the Soviet effort he observed in Novosibirsk in the field of stabilized lasers, laser frequency measurements, and the scientific application of both of these is about seven times greater than that currently in progress at NBS and that their accomplishments probably surpass ours in several areas. NBS is currently employing some techniques that were originally suggested by the Novosibirsk group.

Dr. Kharlamov of the Soviet Academy spent most of his three-months' visit at NBS developing computer algorithms and programs for NBS data logging systems. He wrote and left with NBS a set of four useful computer programs that we now use in connection with data acquisition and processing in certain experimental areas connected with our diode laser spectrometer.

As a result of Dr. Givargizov's visit to NBS, we gained possession of a worthwhile collection of whisker crystal specimens that he brought with him from the USSR and that will benefit our future work.

Of course, NBS feels that it has not always received the full scope of technical benefit that it expected. However, these cases relate to only portions of the originally proposed programs, the remaining portions of which were achieved to our satisfaction.

Potential for Technology Loss to the United States: At the very beginning of implementation of the MoC, the Director of NBS established an internal NBS Coordinating Council to approve and monitor joint activities under the MoC to ensure that these activities provided technical benefits to NBS and the United States. The Director serves as the Chairman of this Council. In its appraisal of applications under the MoC, the Council pays particular attention to the questions of reciprocity, mutual benefit, scientific soundness, and any potential for significant technological loss to the United States. Subject areas are limited to those considered to be basic rather than applied research. In addition, before responding to the Soviet Academy, NBS routinely transmits Soviet applications to the State Department and to the Committee on Exchanges (COMEX) to obtain a thorough inter-agency appraisal of any potential technological loss. As a result of these evaluations and other internal considerations (such as whether the proposed program coincides with areas of current NBS interests), NBS has either rejected or modified several proposed Soviet visits. (No proposed visit by NBS scientists to the USSR has been rejected by the Soviet side.) While the Soviet visitors are in residence at NBS, care is taken to limit their access to the agreed areas only.

Cost Savings Achieved through Implemenation of the MoC: As noted above, the budgetary outlay in the implementation of the MoC is quite modest in comparison with the technical benefits achieved. Technical benefits translate directly into cost savings through contributions to our own domestic objectives. One example of cost savings and avoidance of duplication of effort has already been mentioned--the joint production of a compilation of critically evaluated thermophysical data that will be a major publication of the U.S. National Standard Reference Data System that is overseen by NBS. This effort also includes exchanges of bibliographic references, which serves to strengthen the NBS knowledge of the availability of Soviet data in this field--data that might otherwise have been overlooked. During the past 2 years, the Soviet side has provided NBS with about 60,000 microfiche images containing such information, and NBS has provided the Soviet side with an equivalent number of references to U.S. literature.

NBS Recommendation: In recent months, NBS has received several inquiries from Soviet visitors and from officials in Moscow regarding NBS wishes to renew the agreement. At a reception in early 1983 at the Soviet Embassy in Washington, Academy Vice President Velikhov suggested that the Academy would be interested in an extension if NBS were.

In the judgment of NBS participants, the NBS/ASUSSR program of collaboration (1) has been of significant benefit to the technical objectives of NBS and (2) has provided a means of acquiring information on scientific programs within USSR laboratories that is not available from any other source. We recommend, therefore, that if there are no overriding objections on foreign policy grounds, authorization be given to NBS to propose to the USSR Academy of Sciences that the existing Memorandum on Cooperation be renewed for another five-year period.

Attachments

cc:
L. Starbird

$3p^6\ 3d^8$–$3p^5\ 3d^9$ transitions in Sr XIII, Y XIV, Zr XV, Nb XVI, and Mo XVII

Joseph Reader and Aleksandr Ryabtsev*

National Bureau of Standards, Washington, D.C. 20234

Received September 29, 1980

The $3p^6\ 3d^8$–$3p^5\ 3d^9$ transitions in Sr XIII, Y XIV, Zr XV, Nb XVI, and Mo XVII have been newly measured by means of a low-inductance vacuum spark and a 10.7-m grazing-incidence spectrograph. The measurements have led to an improved analysis of this complex transition group in these ions. All levels of the combining configurations have been established. The energy parameters determined from least-squares fits to the observed levels are compared with Hartree–Fock calculations. The effective interaction $\alpha L(L+1)$ for the $3p^6\ 3d^8$ configuration decreases markedly with increasing ionization. The effective electrostatic interactions $D^1(3p3d)$ and $X^2(3p3d)$ for the $3p^5\ 3d^9$ configuration are practically constant through the sequence.

Ions of the isoelectronic sequence Sr XIII–Mo XVII have the ground configuration $3p^6\ 3d^8$. The lowest excited configuration is $3p^5\ 3d^9$. In each ion the $3p^6\ 3d^8$–$3p^5\ 3d^9$ transitions form a complex group of lines that span a region of only about 18 Å. This region also contains complex spectra that are due to $3p^6\ 3d^n$–$3p^5\ 3d^{n+1}$ transitions of higher stages of ionization. The investigation of these transition groups thus requires selective excitation and high resolution. A photograph of this complex spectral region for Mo, as observed in spectra of the DITE Tokamak and a laser-produced plasma, has been given by Mansfield *et al.*[1]

The $3p^6\ 3d^8$–$3p^5\ 3d^9$ transitions in Y XIV, Zr XV, Nb XVI, and Mo XVII were investigated recently by Bogdanovichene *et al.*[2] They used a low-inductance vacuum spark together with 2- and 3-m grazing-incidence spectrographs to identify about 25 lines in each spectrum. From these identifications most of the energy levels of the two configurations were established. In a parallel investigation, Burkhalter *et al.*[3] used a low-inductance vacuum spark and a 2.2-m grazing-incidence spectrograph to identify 14 prominent $3p^6\ 3d^8$–$3p^5\ 3d^9$ transitions in Mo XVII.

In the present work we observed spectra of strontium, yttrium, zirconium, niobium, and molybdenum with a low-inductance vacuum spark and the 10.7-m grazing incidence spectrograph at the National Bureau of Standards (NBS). With these observations we were able to extend and partially revise the analyses of the ions Y XIV–Mo XVII as well as to provide the first spectral data for Sr XIII. About 40 lines have been identified in each spectrum. All levels of the $3p^6\ 3d^8$ and $3p^5\ 3d^9$ configurations have now been established for these ions.

EXPERIMENT

The measurements were taken largely from spectrograms made in connection with recent investigations of several highly charged copperlike and zinclike ions.[4–8] These observations were made with the NBS 10.7-m spectrograph at an angle of incidence of 80°. The grating had 1200 lines/mm. At this angle of incidence the lowest wavelength that could be recorded was about 70 Å. As several important transitions for the present ions were expected to lie below 70 Å, new exposures were taken on the 10.7-m spectrograph at an angle of incidence of 85°. At this angle, spectra could be observed to about 33 Å. Wavelength-calibration procedures and further experimental details are given in Refs. 4–8.

The wavelengths, intensities, and classifications of the $3p^6\ 3d^8$–$3p^5\ 3d^9$ transitions of Sr XIII–Mo XVII obtained in the present work are given in Table 1. The uncertainty of the wavelengths is ±0.005 Å. For perturbed lines the uncertainty is ±0.010 Å. The intensities are visual estimates of photographic blackening. As noted in the table, many of the values represent new measurements for lines given originally in Refs. 2 and 3.

ANALYSIS OF THE SPECTRA

To extend the analyses we first made least-squares fits for the most-reliably determined $3p^6\ 3d^8$ and $3p^5\ 3d^9$ levels.[2] The $3p^6\ 3d^8$ levels included $^3F_{2,3,4}$, $^3P_{1,2}$, and $^1D_2$. The $3p^5\ 3d^9$ levels included $^3F_{2,3,4}$, $^3P_{1,2}$, $^3D_{1,2,3}$, and $^1D_2$. These levels were confirmed by additional combinations found in the present observations. The levels $3p^6\ 3d^8\ ^3P_0$, $^1G_4$, $^1S_0$, and $3p^5\ 3d^9\ ^3P_0$, $^1F_3$, and $^1P_1$, which previously[2] were either doubtful or missing altogether in some ions, were thus excluded. Initial values for the parameters were taken from Hartree–Fock (HF) calculations made with the computer program of Froese-Fischer.[9] No effective interactions were included. These calculations proved to be satisfactory from the standpoint of regularity of parameter values and mean errors. The predicted level values were thus adopted as a basis for further analysis of the spectra.

$3p^5\ 3d^9\ ^1P_1$

This level had been established by a single transition in each ion, $^1D_2$–$^1P_1$. Our new low-wavelength data provided the $^3P_2$–$^1P_1$ combinations, confirming the previous identifications in Y, Zr, and Mo. For Nb XVI the previous $^1D_2$–$^1P_1$ identification (70.474 Å) was replaced by a line at 70.718 Å, resulting in a revised value for $3p^5\ 3d^9\ ^1P_1$.

Reprinted from **Journal of the Optical Society of America,**
Vol. 71, page 231, March, 1981

$3p^6\,3d^8\,{}^1S_0$

This level was based on the single transition $^1S_0$–$^1P_1$. The identification was listed[2] as doubtful in Y and Zr and was absent in Nb and Mo. We have now replaced these identifications with those given in Table 1, which includes values for Nb and Mo as well. These lines were the most prominent unidentified lines in the expected region and, although there are no confirming transitions, there is little doubt that the identifications are correct. They are strongly supported by the least-squares calculations.

$3p^6\,3d^8\,{}^1G_4$ and $3p^5\,3d^9\,{}^1F_3$

The $^1G_4$–$^1F_3$ transition is easily identified as an intense line on the low-wavelength side of the transition group.[2,3] It has the highest predicted line strength within the present array. In Ref. 2 these levels were connected to the main body of levels through the single transition $^1G_4$–$^3D_3$. We have now replaced the $^1G_4$–$^3D_3$ identifications with those given in Table 1. This in turn revises the $^1G_4$ and $^1F_3$ level values. The new values are confirmed by the four additional combinations, $^3F_3$–$^1F_3$, $^3F_2$–$^1F_3$, $^1D_2$–$^1F_3$, and $^1G_4$–$^3F_3$. The line identified as $^1G_4$–$^3D_3$ in Y XIV was previously identified as $^3P_1$–$^3P_0$.

Table 1. Observed $3p^6\,3d^8$–$3p^5\,3d^9$ Transitions in Sr XIII, Y XIV, Zr XV, Nb XVI, and Mo XVII [a]

Transition	Sr XIII		Y XIV		Zr XV		Nb XVI		Mo XVII	
	λ(Å)	Int.	λ(Å)	Int.	λ(Å)	Int.	λ(Å)	Int.	λ(Å)	Int.
$3p^6\,3d^8\,{}^3F_3$–$3p^5\,3d^9\,{}^1F_3$			76.229	10	72.455	10	68.989	10	65.770	4
$^3F_2$–$3p^5\,3d^9\,{}^1F_3$			76.506	1h	72.692	1h	69.174	2	65.891	1h
$^3P_2$–$3p^5\,3d^9\,{}^1P_1$			77.268	25	73.239	15	69.540	15	66.100	3
$^1D_2$–$3p^5\,3d^9\,{}^1P_1$	82.758	75	78.395[b]	50p	74.395[b]	40	70.718	40	67.302[c]	15
$^1D_2$–$3p^5\,3d^9\,{}^1F_3$			78.813	10	74.966	3	71.448	5	68.188	3h
$^1G_4$–$3p^5\,3d^9\,{}^1F_3$	83.656	2000	79.338[b]	3000	75.385[b]	2000	71.759	1200	68.390[c]	800
$^3F_3$–$3p^5\,3d^9\,{}^3P_2$	85.311	120	80.714[b]	150	76.509[b]	70	72.656	100	69.088	30
$^3F_2$–$3p^5\,3d^9\,{}^3P_2$			81.030[b]	20	76.777	10	72.870	5		
$^3P_2$–$3p^5\,3d^9\,{}^3P_2$			82.334	50	78.006[b]	20	74.049	20	70.386[c]	15
$^3F_3$–$3p^5\,3d^9\,{}^3F_2$			82.628	5			74.132	2	70.367	3
$^3F_2$–$3p^5\,3d^9\,{}^3F_2$	87.831	100	82.963[b]	120	78.483[b]	30	74.352	20	70.494	5
$^3P_1$–$3p^5\,3d^9\,{}^3P_2$	88.151	200	83.397[b]	140	79.046[b]	70	75.060	70	71.359[c]	30
$^1D_2$–$3p^5\,3d^9\,{}^3P_2$			83.614	70	79.318	15			71.750	5
$^1S_0$–$3p^5\,3d^9\,{}^1P_1$	88.631	70	83.970	50	79.689	30	75.754	20	72.092	20
$^3F_2$–$3p^5\,3d^9\,{}^3D_1$	88.568	500	84.211[b]	200	80.247[b]	250	76.631[b]	120	73.289[c]	200
$^3F_4$–$3p^5\,3d^9\,{}^3D_3$	88.754	800	84.266[b]	400	80.176[b]	400	76.442[b]	300	72.990[c]	300
$^3P_2$–$3p^5\,3d^9\,{}^3F_2$			84.326	25	79.766	2h	75.590	20p	71.705	7
$^3F_3$–$3p^5\,3d^9\,{}^3D_3$	89.797	200	85.372[b]	160	81.350[b]	250	77.685[b]	120	74.306[c]	200
$^3P_2$–$3p^5\,3d^9\,{}^3D_1$			85.618[b]	25			77.949[b]	30	74.600	5
$^1D_2$–$3p^5\,3d^9\,{}^3F_2$	90.618	150	85.673[b]	150	81.140[b]	200	76.980[b]	120	73.122[c]	150
$^3P_0$–$3p^5\,3d^9\,{}^3D_1$	91.253	60	86.767[b]	70	82.696[b]	25	78.986[b]	40	75.580	15
$^3F_3$–$3p^5\,3d^9\,{}^3D_2$	91.481	500	87.009[b]	400	82.948	300	79.241	500	75.840[b]	150
$^3P_2$–$3p^5\,3d^9\,{}^3D_3$	91.757	100	87.184[b]	100	83.048[b]	100	79.284[b]	50p	75.816	15
$^3F_4$–$3p^5\,3d^9\,{}^3F_3$	92.664	600	87.984[b]	600	83.727[b]	700	79.839[b]	500	76.269[c]	600
$^3P_2$–$3p^5\,3d^9\,{}^3P_1$	92.734	150	88.186[b]	140	84.061[b]	100	80.298[b]	150	76.863[b]	200h
$^1D_2$–$3p^5\,3d^9\,{}^3D_3$			88.623	5	84.534	2			77.396	5p
$^3P_2$–$3p^5\,3d^9\,{}^3D_2$	93.517	150	88.893[b]	150	84.708[b]	100	80.890[b]	80	77.410[b]	20
$^3P_1$–$3p^5\,3d^9\,{}^3P_0$	93.772	80	89.190[d,e]	600	85.031[b]	200	81.213[e]	80	77.727	30
$^3F_3$–$3p^5\,3d^9\,{}^3F_3$	93.800	100	89.190[d,e]	600	85.011	70	81.202	100	77.706	20
$^1G_4$–$3p^5\,3d^9\,{}^3D_3$	93.967	50	89.287[d]	75	85.064	30	81.213[e]	80	77.666[b]	30
$^3P_0$–$3p^5\,3d^9\,{}^3P_1$			89.408[d,e]	150	85.236	20	81.412[d]	20	77.898	15
$^3P_1$–$3p^5\,3d^9\,{}^3P_1$			89.408[b,e]	150	85.269[b]	40	81.489	80	78.019[b]	40
$^1D_2$–$3p^5\,3d^9\,{}^3D_2$	94.955	50	90.389[b]	120	86.256[b]	70	82.495[b]	50	79.062[b]	100
$^3F_4$–$3p^5\,3d^9\,{}^3F_4$	95.528	1500	90.871[b]	1500	86.630[b]	1500	82.749[b]	1500	79.186[c]	1500
$^3F_3$–$3p^5\,3d^9\,{}^1D_2$			90.967	5			82.993	50bl	79.532	5
$^3P_2$–$3p^5\,3d^9\,{}^3F_3$			91.177	5h			82.945	2	79.359	5
$^3F_2$–$3p^5\,3d^9\,{}^1D_2$	95.998	400	91.371[b]	600	87.147[b,g]	600	83.275[b]	600	79.711[c]	700
$^3F_3$–$3p^5\,3d^9\,{}^3F_4$	96.739	200[f]	92.160	40	88.006[b]	20h	84.211[b]	100	80.734	30
$^1D_2$–$3p^5\,3d^9\,{}^3F_3$	97.450	100	92.749	25	88.486	20	84.619	40	81.080	20p
$^3P_2$–$3p^5\,3d^9\,{}^1D_2$	97.766	400	93.031[b]	400	88.732[b]	300	84.823[b]	150	81.261[b]	100
$^1G_4$–$3p^5\,3d^9\,{}^3F_3$			93.478	15	89.069	20	85.058	10	81.382	20
$^3P_1$–$3p^5\,3d^9\,{}^1D_2$			94.390	10	90.080	10	86.154	30	82.556	20
$^1D_2$–$3p^5\,3d^9\,{}^1D_2$	99.341	100	94.671[b]	100	90.434[b]	100	86.586[b]	30	83.079[b]	50

[a] Symbols: bl, blend of two lines; h, hazy; p, perturbed by close line.
[b] Present value for line given originally by Bogdanovichene *et al.*, Ref. 2.
[c] Present value for line given originally by Bogdanovichene *et al.*, Ref. 2, and by Burkhalter *et al.*, Ref. 3.
[d] Present value for line given originally by Bogdanovichene *et al.*, Ref. 2, revised classification.
[e] Doubly classified.
[f] Blended with 96.731 Å of Ti. (The Sr exposures were made with an anode of Sr and a cathode of Ti.)
[g] Blended with a line of Zr XII; see Ref. 7.

Table 2. Energy Levels (in cm^{-1}) of the $3p^6\,3d^8$ and $3p^5\,3d^9$ Configurations of Sr XIII, Y XIV, Zr XV, Nb XVI, and Mo XVII

Configuration	Term	J	Sr XIII[a]	Y XIV	Zr XV	Nb XVI	Mo XVII
$3p^6\,3d^8$	^3F	4	0	0	0	0	0
		3	13 080	15 380	18 030	20 960	24 250
		2	18 000	20 230	22 560	24 890	27 030
	^3P	2	36 850	39 760	43 080	46 840	51 000
		0	51 230	55 230	59 470	63 830	68 350[a]
		1	50 840	55 240	59 940	65 020[a]	70 310
	^1D	2	53 040	58 380	64 280	70 790	77 960
	^1G	4	62 500	66 780[a]	71 660[a]	76 870[a]	82 420[a]
	^1S	0	133 120	143 060[a]	153 590[a]	164 790[a]	176 700[a]
$3p^5\,3d^9$	^3F	4	1 046 800	1 100 460	1 154 330	1 208 470	1 262 860
	^1D	2	1 059 690	1 114 670	1 170 060	1 225 740	1 281 600
	^3F	3	1 079 180	1 136 550	1 194 370	1 252 520	1 311 160
	^3D	2	1 106 180	1 164 700	1 223 610	1 282 970	1 342 800
	^3P	1	1 115 200	1 173 720	1 232 700	1 292 180	1 352 050
	^3P	0	1 117 250	1 176 440[a]	1 235 980[a]	1 296 360[a]	1 356 860[a]
	^3D	3	1 126 700	1 186 740	1 247 240	1 308 200	1 370 010
	^3D	1	1 147 080	1 207 730	1 268 720	1 329 840	1 391 470
	^3F	2	1 156 570	1 225 610	1 296 720	1 369 820	1 445 570
	^3P	2	1 185 260	1 254 340	1 325 040	1 397 270[a]	1 471 690
	^1F	3	1 257 880	1 327 220[a]	1 398 200[a]	1 470 450[a]	1 544 660[a]
	^1P	1	1 261 390	1 333 960	1 408 460	1 484 850[a]	1 563 830

[a] New level; all levels for Sr XIII are new.

$3p^5\,3d^9\,{}^3P_0$

This level makes only one combination within the present array, $^3P_1$–$^3P_0$. Although this transition is expected to be fairly strong, its identification is made difficult by the complexity of the spectrum in the expected region. Based on the present observations and calculations, we propose the new identifications for this transition given in Table 1. In Zr and Mo there is not much doubt about the assignments, because there is only one clear choice. In Y and Nb the proposed lines represent blends with other transitions of the same array. However, these identifications are well supported by isoelectronic regularities. The evidence for a blend in Y is particularly strong because there is no other possible choice within a reasonable distance of the predicted position and, furthermore, the other member of the blend, $^3F_3$–$^3F_3$, appears to be anomalously strong compared with its appearance elsewhere in the sequence.

$3p^6\,3d^8\,{}^3P_0$

This level can make three transitions, of which two, $^3P_0$–$^3P_1$ and $^3P_0$–$^3D_1$, are expected to be reasonably strong and one, $^3P_0$–$^1P_1$, is expected to be weak. In Ref. 2, values for $^3P_0$ were

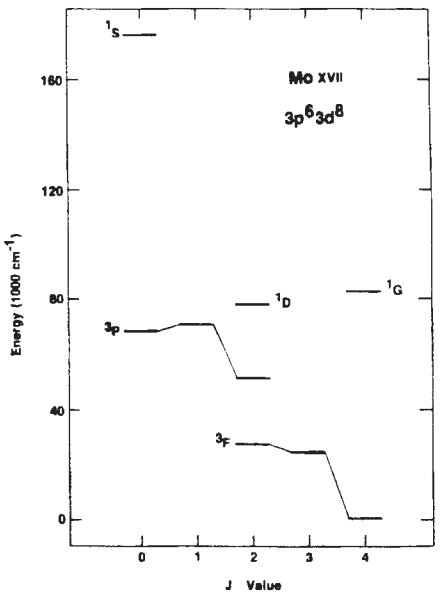

Fig. 1. Structure of the $3p^6\,3d^8$ configuration of Mo XVII.

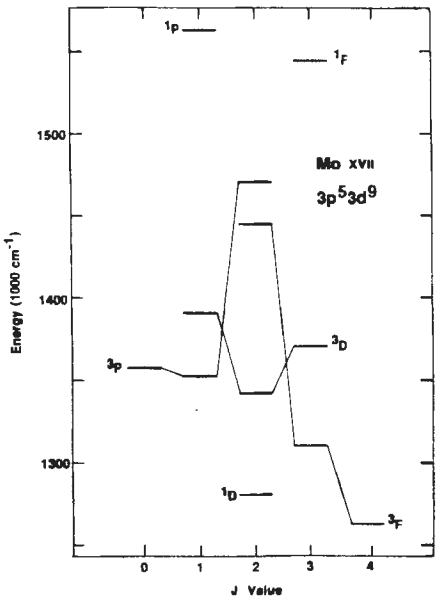

Fig. 2. Structure of the $3p^5\,3d^9$ configuration of Mo XVII. Levels are grouped into LS terms.

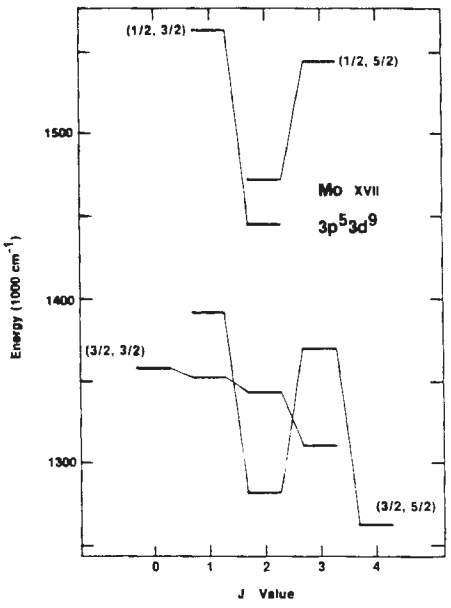

Fig. 3. Structure of the $3p^5\ 3d^9$ configuration of Mo XVII. Levels are grouped into jj terms.

given for Y, Zr, and Nb based on the single transition $^3P_0$–$^3D_1$. No value was given for Mo. We have now observed the $^3P_0$–$^3D_1$ as well as the $^3P_0$–$^3P_1$ transition for the present ions, confirming the previous identifications and providing values for Mo. In Y the $3p^6\ 3d^8\ ^3P_0$ and $^3P_1$ levels are nearly coincident and the $^3P_0$–$^3P_1$ and $^3P_1$–$^3P_1$ transitions thus cannot be resolved. Our value for $^3P_0$–$^3D_1$ in Mo replaces the identification for this transition given in Ref. 3.

Sr XIII

The spectra for this ion were relatively weak, but with the help of isoelectronic regularities the principal lines of the array and all of the levels could in fact be located. The presence of $^3P_1$–$^3P_0$ as a fairly strong line in Sr further supports the proposed blend of $^3P_1$–$^3P_0$ and $^3F_3$–$^3F_3$ in Y.

Finally, we confirm the value for $^3F_3$–$^3D_2$ of Mo XVII given in Ref. 2 (75.843 Å), compared with the value given in Ref. 3 (75.624 Å). The resulting levels are supported by several other combinations.

The values of the energy levels are given in Table 2. These values were determined by an optimization procedure[10] that minimizes the differences between the observed and calculated wave numbers. The uncertainty of the level values is about $\pm 50\ \text{cm}^{-1}$.

Table 3. Energy Parameters (in cm^{-1}) and Mean Errors Δ of Least-Squares Fits for the $3p^6\ 3d^8$ Configurations of Sr XIII, Y XIV, Zr XV, Nb XVI, and Mo XVII.[a]

Ion	Parameter	HF	Fitted	Fitted–HF
Sr XIII	E_{av}	36 440	34 031 ± 63	
	$F^2(3d3d)$	214 978	194 218 ± 513	0.903 ± 0.002
	$F^4(3d3d)$	136 981	115 570 ± 468	0.844 ± 0.003
	$\alpha(3d3d)$		203 ± 12	
	ζ_{3d}	6 133	6 207 ± 74	1.012 ± 0.012
	Δ		167	
Y XIV	E_{av}	39 578	37 009 ± 61	
	$F^2(3d3d)$	225 641	204 477 ± 496	0.906 ± 0.002
	$F^4(3d3d)$	143 929	123 560 ± 456	0.858 ± 0.003
	$\alpha(3d3d)$		171 ± 11	
	ζ_{3d}	7 196	7 226 ± 70	1.004 ± 0.010
	Δ		161	
Zr XV	E_{av}	42 883	40 323 ± 82	
	$F^2(3d3d)$	236 241	215 429 ± 678	0.912 ± 0.003
	$F^4(3d3d)$	150 838	131 717 ± 627	0.873 ± 0.004
	$\alpha(3d3d)$		156 ± 15	
	ζ_{3d}	8 388	8 365 ± 92	0.997 ± 0.011
	Δ		218	
Nb XVI	E_{av}	46 430	43 903 ± 103	
	$F^2(3d3d)$	246 787	226 602 ± 847	0.918 ± 0.003
	$F^4(3d3d)$	157 711	140 221 ± 789	0.889 ± 0.005
	$\alpha(3d3d)$		138 ± 19	
	ζ_{3d}	9 717	9 641 ± 108	0.992 ± 0.011
	Δ		272	
Mo XVII	E_{av}	50 238	47 735 ± 118	
	$F^2(3d3d)$	257 286	238 019 ± 975	0.925 ± 0.004
	$F^4(3d3d)$	164 554	149 180 ± 918	0.907 ± 0.006
	$\alpha(3d3d)$		123 ± 22	
	ζ_{3d}	11 195	11 080 ± 117	0.990 ± 0.010
	Δ		312	

[a] The value of E_{av} listed in the HF column is that obtained by diagonalizing the energy matrix with the HF parameters, $^3F_4$ level set at zero.

Table 4. Percentage Compositions for the $3p^6\,3d^8$ Levels of Sr XIII, Zr XV, and Mo XVII

J	Term	Percentage Composition (LS)
0	^3P	96, 95, 93% ^3P + 4, 5, 7% ^1S
	^1S	96, 95, 93% ^1S + 4, 5, 7% ^3P
1	^3P	100, 100, 100% ^3P
2	^3F	79, 69, 57% ^3F + 19, 27, 34% ^1D + 2, 4, 9% ^3P
	^3P	47, 52, 55% ^3P + 37, 24, 12% ^1D + 16, 24, 33% ^3F
	^1D	45, 50, 52% ^1D + 51, 43, 37% ^3P + 4, 7, 11% ^3F
3	^3F	100, 100, 100% ^3F
4	^3F	99, 99, 98% ^3F + 1, 1, 2% ^1G
	^1G	99, 99, 98% ^1G + 1, 1, 2% ^3F

The levels of the $3p^6\,3d^8$ configuration of Mo XVII are plotted in Fig. 1. Although a few distortions are evident, the levels can be designated fairly well in the LS scheme. The $3p^5\,3d^9$ levels of Mo XVII are plotted with LS designations in Fig. 2 and with jj designations in Fig. 3. Clearly, neither scheme is satisfactory. Although, as discussed below, the coupling is a little closer to jj than to LS, we have retained LS designations for the levels in order to facilitate comparison with Ref. 2, in which LS designations are used throughout.

THEORETICAL INTERPRETATION

The results of fitting the theoretical energy parameters to the observed $3p^6\,3d^8$ level values by least-squares calculations are

Table 5. Energy Parameters (in cm^{-1}) and Mean Errors Δ of Least-Squares Fits for the $3p^5\,3d^9$ Configurations of Sr XIII, Y XIV, Zr XV, Nb XVI, and Mo XVII

Ion	Parameter	HF	Fitted	Fitted–HF
Sr XIII	E_{av}	1 112 692	1 131 577 ± 46	
	$F^2(3p3d)$	202 415	193 004 ± 546	0.954 ± 0.003
	$G^1(3p3d)$	235 516	199 797 ± 237	0.848 ± 0.001
	$G^3(3p3d)$	150 323	141 352 ± 456	0.940 ± 0.003
	$D^1(3p3d)$		−13 736 ± 412	
	$X^2(3p3d)$		−6 063 ± 569	
	ζ_{3p}	55 838	58 728 ± 87	1.052 ± 0.002
	ζ_{3d}	6 096	5 984 ± 60	0.982 ± 0.010
	Δ		148	
Y XIV	E_{av}	1 166 512	1 192 951 ± 60	
	$F^2(3p3d)$	210 891	201 963 ± 736	0.958 ± 0.003
	$G^1(3p3d)$	244 026	208 819 ± 312	0.856 ± 0.001
	$G^3(3p3d)$	156 264	147 262 ± 617	0.942 ± 0.004
	$D^1(3p3d)$		−13 522 ± 544	
	$X^2(3p3d)$		−5 883 ± 743	
	ζ_{3p}	63 880	67 429 ± 110	1.056 ± 0.002
	ζ_{3d}	7 152	7 004 ± 78	0.979 ± 0.011
	Δ		193	
Zr XV	E_{av}	1 220 111	1 255 174 ± 83	
	$F^2(3p3d)$	219 314	210 733 ± 1056	0.961 ± 0.005
	$G^1(3p3d)$	252 433	218 008 ± 438	0.864 ± 0.002
	$G^3(3p3d)$	162 142	153 534 ± 889	0.947 ± 0.005
	$D^1(3p3d)$		−13 722 ± 764	
	$X^2(3p3d)$		−6 304 ± 1038	
	ζ_{3p}	72 760	77 094 ± 148	1.060 ± 0.002
	ζ_{3d}	8 335	8 162 ± 107	0.979 ± 0.013
	Δ		267	
Nb XVI	E_{av}	1 274 595	1 318 169 ± 117	
	$F^2(3p3d)$	227 690	219 792 ± 1527	0.965 ± 0.007
	$G^1(3p3d)$	260 752	226 922 ± 622	0.870 ± 0.002
	$G^3(3p3d)$	167 965	159 526 ± 1295	0.950 ± 0.008
	$D^1(3p3d)$		−13 771 ± 1085	
	$X^2(3p3d)$		−7 039 ± 1469	
	ζ_{3p}	82 533	87 640 ± 204	1.062 ± 0.002
	ζ_{3d}	9 657	9 475 ± 148	0.981 ± 0.015
	Δ		374	
Mo XVII	E_{av}	1 328 831	1 382 222 ± 132	
	$F^2(3p3d)$	236 026	228 252 ± 1772	0.967 ± 0.008
	$G^1(3p3d)$	268 994	235 911 ± 713	0.877 ± 0.003
	$G^3(3p3d)$	173 740	165 595 ± 1518	0.953 ± 0.009
	$D^1(3p3d)$		−14 052 ± 1242	
	$X^2(3p3d)$		−6 745 ± 1679	
	ζ_{3p}	93 255	99 559 ± 226	1.068 ± 0.002
	ζ_{3d}	11 125	10 918 ± 166	0.981 ± 0.015
	O		422	

Table 6. Percentage Compositions for the $3p^5\,3d^9$ Levels of Sr XIII, Zr XV, and Mo XVII

J	Term	Percentage jj	Percentage Composition (LS)
0	^3P	100, 100, 100% (3/2,3/2)	100, 100, 100% ^3P
1	^3P	81, 78, 75% (3/2,3/2)	84, 85, 86% ^3P + 16, 14, 12% ^3D + 0, 1, 2% ^1P
	^3D	63, 66, 66% (3/2,5/2)	68, 65, 63% ^3D + 22, 27, 32% ^1P + 10, 8, 5% ^3P
	^1P	80, 85, 89% (1/2,3/2)	78, 72, 66% ^1P + 16, 20, 25% ^3D + 6, 8, 9% ^3P
2	^1D	70, 73, 77% (3/2,5/2)	75, 74, 73% ^1D + 17, 15, 14% ^3F + 8, 10, 12% ^3P
	^3D	67, 72, 76% (3/2,3/2)	45, 49, 51% ^3D + 31, 31, 31% ^3P + 23, 20, 18% ^3F
	^3F	93, 96, 98% (1/2,3/2)	59, 63, 66% ^3F + 19, 20, 20% ^1D + 12, 9, 7% ^3D
	^3P	97, 98, 98% (1/2,5/2)	51, 51, 51% ^3P + 43, 42, 41% ^3D + 5, 6, 6% ^1D
3	^3F	66, 63, 60% (3/2,3/2)	79, 72, 65% ^3F + 21, 27, 34% ^3D
	^3D	66, 62, 58% (3/2,5/2)	75, 66, 57% ^3D + 17, 22, 28% ^3F + 8, 12, 15% ^1F
	^1F	62, 67, 71% (1/2,5/2)	91, 88, 84% ^1F + 5, 7, 9% ^3D + 4, 5, 7% ^3F
4	^3F	100, 100, 100% (3/2,5/2)	100, 100, 100% ^3F

given in Table 3. The HF values of the parameters are also given here. The parameter α for the effective electrostatic interaction $\alpha L(L+1)$ is small but well defined. Its introduction into the calculation reduced the mean error of the fit considerably; for Y XIV, for example, the mean error decreased from 1300 to 161 cm^{-1}. The present values of α are consistent with the value of 108 cm^{-1} obtained by Podobedova *et al.*[11] for the isoelectronic ion Ge VII. A value for α of 48 cm^{-1} was obtained by Meinders[12] for Cu IV, but this fit included two additional effective interactions, so a direct comparison may not be valid. Interestingly, for the present series of atoms, α decreases significantly with increasing ionization.

The ratios of the fitted values of the parameters to the HF values shown in Table 3 are generally close to unity. This is surprising because the HF calculation[9] does not include the effects of relativity. The ratios vary smoothly through the sequence.

Table 7. Differences between Observed Level Values and Those Calculated with the Fitted Values of the Parameters for the $3p^6\,3d^8$ and $3p^5\,3d^9$ Configurations of Sr XIII, Y XIV, Zr XV, Nb XVI, and Mo XVII (in cm^{-1})

Configuration	J	Term	Sr XIII	Y XIV	Zr XV	Nb XVI	Mo XVII
$3p^6\,3d^8$	0	^3P	110	100	110	30	10
		^1S	−20	10	30	40	70
	1	^3P	−110	10	70	190	220
	2	^3F	220	220	210	180	−10
		^3P	80	−110	−220	−250	−230
		^1D	−80	−130	−180	−240	−290
	3	^3F	−90	30	150	270	420
	4	^3F	−130	−110	−160	−180	−150
		^1G	0	−10	−20	−20	−40
$3p^5\,3d^9$	0	^3P	10	100	90	160	120
	1	^3P	−110	−240	−280	−410	−370
		^3D	100	−10	−60	−150	−220
		^1P	−30	0	30	70	120
	2	^1D	10	20	30	50	60
		^3D	80	150	230	310	340
		^3F	−70	−110	−170	−240	−290
		^3P	90	110	160	200	220
	3	^3F	100	120	200	250	330
		^3D	−190	−140	−220	−270	−360
		^1F	20	10	30	40	70
	4	^3F	−30	−40	−40	−20	0

The percentage compositions for the $3p^6\,3d^8$ configurations of Sr XIII, Zr XV, and Mo XIII are given in Table 4. As already noted, the coupling is close to LS, although the $^3P_2$ and $^1D_2$ states are strongly admixed.

The parameters for the $3p^5\,3d^9$ configurations are given in Table 5. The fitted–HF ratios are again close to unity and vary smoothly through the sequence. The parameters $D^1(3p3d)$ and $X^2(3p3d)$ for the direct and exchange effective electrostatic interactions[13] are well defined. Of the two, the direct interaction $D^1(3p3d)$ is the more important. Its introduction into the calculation reduced the mean error for Y XIV from 2300 to 700 cm^{-1}. Addition of $X^2(3p3d)$ further reduced the mean error to 193 cm^{-1}. [When $X^2(3p3d)$ is added alone, the mean error is reduced only to 2200 cm^{-1}.] These parameters are thus significant. Their values are nearly constant through the sequence.

The percentage compositions for the $3p^5\,3d^9$ configurations of Sr XIII, Zr XV, and Mo XVII are given in Table 6. As already mentioned, the major components in the jj scheme are generally higher than in the LS scheme. In the jl scheme the major component percentages were found to be a little lower on the average than in the jj scheme.

The differences between the observed level values and those calculated with the fitted values of the parameters are given in Table 7. The differences generally vary smoothly, although there are a few irregularities, such as for $3p^6\,3d^8\,^3F_2$ and $^3P_2$. In view of the uncertainties of the level values, we do not consider these irregularities to be significant.

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$3d$–$4p$ Transitions in the zinclike and copperlike ions Y X, XI; Zr XI, XII; Nb XII, XIII; and Mo XIII, XIV

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Lines occurring as satellites on the long-wavelength side of the $3d^{10}$–$3d^9 4p$ resonance lines of Ni-like ions have been investigated with a low-inductance vacuum spark and a 10.7-m spectrograph for the elements Y, Zr, Nb, and Mo. The lines are interpreted as $3d^{10}4s$–$3d^9 4s4p$ and $3d^{10}4p$–$3d^9 4p^2$ transitions in the Cu-like ions Y XI, Zr XII, Nb XIII, and Mo XIV and $3d^{10}4s^2$–$3d^9 4s^2 4p$ transitions in the Zn-like ions Y X, Zr XI, Nb XII, and Mo XIII. The spectra of the Cu-like ions were interpreted by generalized least-squares fits for the energy levels of the sequence of four ions. Thirty-nine levels of $3d^9 4s4p$ were interpreted simultaneously with a root-mean-square deviation of 122 cm^{-1}; forty-four levels of $3d^9 4p^2$ were interpreted in the same way with a root-mean-square deviation of 200 cm^{-1}. Line identifications and energy levels were obtained for the $3d^{10}7p$ configuration of the Cu-like ions Y XI–Mo XIV.

The use of highly ionized molybdenum for plasma diagnosis in controlled-fusion research has stimulated spectroscopic investigations of this element in recent years. As a member of the Cu I isoelectronic sequence, Mo XIV has the ground configuration $3d^{10}4s$. Its one-electron spectrum and those of the neighboring members of the sequence Y XI, Zr XII, and Nb XIII have already been well described.[1–4] In a recent description[5] of the spectra of Mo XIII–XVIII from laser-produced plasmas and low-inductance vacuum sparks, satellite lines occurring on the high-wavelength side of the $3d^{10}$–$3d^9 4p$ resonance transitions of the Ni-like ion Mo XV were interpreted as $3d^{10}4s$–$3d^9 4s4p$ transitions of Mo XIV and $3d^{10}4s^2$–$3d^9 4s^2 4p$ transitions of Mo XIII. Unfortunately, three prominent lines near the middle of the satellite group remained unexplained.

In the present work we photographed spectra of Y, Zr, Nb, and Mo on the 10.7-m grazing-incidence spectrograph at the National Bureau of Standards (NBS) and theoretically interpreted the corresponding satellite line groups in each of these spectra. The unexplained lines in Mo were interpreted as $3d^{10}4p$–$3d^9 4p^2$ transitions of Mo XIV.

EXPERIMENT

The experimental material for this work was the same as used for a recent study of $3p^6 3d^8$–$3p^5 3d^9$ transitions of Y XIV, Zr XV, Nb XVI, and Mo XVII.[6] Briefly, the 10.7-m grazing-incidence spectrograph at NBS was used at angles of incidence of 80° and 85° to record spectra from a low-inductance vacuum spark between metallic electrodes. The grating had 1200 lines/mm. The plate factor was about 0.12 Å/mm at the 85° angle of incidence.

LINE IDENTIFICATIONS AND THEORETICAL INTERPRETATION

$3d^{10}4s$–$3d^9 4s4p$ Transitions

As was seen in Mo XIV,[5] the strongest satellite lines are due to $3d^{10}4s$–$3d^9 4s4p$ transitions. We thus interpreted these transitions first. The $3d^9 4s4p$ configuration contains 23 levels, of which eleven have $J = 1/2$ or 3/2 and can therefore combine with $3d^{10}4s\ {}^2S_{1/2}$. Our line identifications were made with the help of theoretical calculations of the $3d^9 4s4p$-level structures and $3d^{10}4s$–$3d^9 4s4p$ line strengths in the four ions that were investigated. Initial energy parameters for the $3d^9 4s4p$ configurations were obtained by Hartree–Fock (HF) calculations.[7] After identifying the strongest and most reliable transitions in each ion, we repeated the calculations with values of the parameters determined from least-squares fits to the observed energy levels. New line identifications were then carried out. In this way, 10 of the 11 possible transitions in each ion could be identified. Only the transition $3d^{10}4s\ {}^2S_{1/2}$–$3d^9(^2D)4s4p(^1P)\ {}^2D^\circ_{3/2}$, which is calculated to be 400 times weaker than the strongest transition of the array, could not be identified. The low calculated line strength for this transition results from the fact that the upper level corresponds to a fairly pure $^2D_{3/2}$ state. The previous[5] identification of this transition in Mo XIV is probably spurious.

The wavelengths and classifications of the identified $3d^{10}4s$–$3d^9 4s4p$ transitions are given in Table 1. The uncertainty of the wavelengths is ±0.005 Å. The intensities are visual estimates of photographic plate blackening. The line identifications are well supported by the calculated line strengths, which predict the observed trends well. Because

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Table 1. Lines Classified as $3d^{10}4s$–$3d^94s4p$ and $3d^{10}4p$–$3d^94p^2$ Transitions in Y XI, Zr XII, Nb XIII, and Mo XIV[a]

Classification	Code	Y XI		Zr XII		Nb XIII		Mo XIV	
		λ (Å)	Int.	λ (Å)	Int.	λ (Å)	Int.	λ (Å)	Int.
$4s\ ^2S_{1/2}$–$(^2D, ^1P)\ ^2P^o_{1/2}$	A	73.639	15	64.466	20	57.001	15	50.788	10
$4p\ ^2P^o_{3/2}$–$(^2D, ^1S)\ ^2D_{5/2}$	a	73.908	2	64.794	1*w*	57.393	2	51.20	1
$4p\ ^2P^o_{1/2}$–$(^2D, ^3P)\ ^4P_{3/2}$	b	74.175?	1			57.187	1		
$4p\ ^2P^o_{1/2}$–$(^2D, ^3P)\ ^2P_{1/2}$	c	74.391	5	65.059	2	57.468	2	51.158	1
$4s\ ^2S_{1/2}$–$(^2D, ^1P)\ ^2P^o_{3/2}$	B	74.456	30	65.200	50	57.662	30	51.398	20
$4p\ ^2P^o_{1/2}$–$(^2D, ^1D)\ ^2D_{3/2}$	d	74.896	8	65.466	5	57.797	3	51.434	1
$4p\ ^2P^o_{3/2}$–$(^2D, ^1D)\ ^2F_{5/2}$	e	74.954	2*p*	65.540	3	57.884	2	51.531	1
$4p\ ^2P^o_{3/2}$–$(^2D, ^3P)\ ^4P_{1/2}$	f			65.609	1				
$4p\ ^2P^o_{3/2}$–$(^2D, ^3P)\ ^4P_{3/2}$	g	75.209	10						
$4p\ ^2P^o_{1/2}$–$(^2D, ^3P)\ ^4F_{3/2}$	h	75.233	15	65.760	10	58.053	10	51.666	5
$4p\ ^2P^o_{3/2}$–$(^2D, ^3P)\ ^2P_{3/2}$	i	75.307	25	65.896	10	58.241	15	51.894	8
$4p\ ^2P^o_{1/2}$–$(^2D, ^1D)\ ^2P_{1/2}$	j			65.816?	1				
$4p\ ^2P^o_{3/2}$–$(^2D, ^3P)\ ^2P_{1/2}$	k	75.438	10	66.029	5	58.362	5	52.00	2*u*
$4p\ ^2P^o_{3/2}$–$(^2D, ^3P)\ ^2D_{5/2}$	l	75.521	35	66.080	20	58.386	20	52.013	10*u*
$4p\ ^2P^o_{1/2}$–$(^2D, ^3P)\ ^2D_{3/2}$	m	75.584	25	66.115	10	58.407	10	52.019	8*u*
$4p\ ^2P^o_{1/2}$–$(^2D, ^3P)\ ^4D_{1/2}$	n	75.945	2	66.327	2				
$4s\ ^2S_{1/2}$–$(^2D, ^3P)\ ^4D^o_{3/2}$	C	76.274	25	66.597	8	58.728	10	52.225	5
$4p\ ^2P^o_{1/2}$–$(^2D, ^1D)\ ^2P_{3/2}$	o	76.283?	2*u*	66.687?	3	58.888*	5	52.415*	2
$4p\ ^2P^o_{3/2}$–$(^2D, ^3P)\ ^4F_{5/2}$	p					58.909	3		
$4p\ ^2P^o_{1/2}$–$(^2D, ^1D)\ ^2S_{1/2}$	q	76.331	10	66.717	5*p*	58.888*	5	52.415*	2
$4p\ ^2P^o_{3/2}$–$(^2D, ^1D)\ ^2P_{1/2}$	r	76.434?	15*l*	66.792?	5				
$4p\ ^2P^o_{1/2}$–$(^2D, ^3P)\ ^4D_{3/2}$	s	76.584?	15						
$4s\ ^2S_{1/2}$–$(^2D, ^3P)\ ^4D^o_{1/2}$	D	76.66	1	66.928	3	59.016	5*w*	52.473	5
$4s\ ^2S_{1/2}$–$(^2D, ^3P)\ ^2P^o_{1/2}$	E	76.843	40	67.121	30	59.214	20	52.687	10
$4s\ ^2S_{1/2}$–$(^2D, ^3P)\ ^2P^o_{3/2}$	F	76.920	50	67.201	50	59.285	40	52.750	20
$4s\ ^2S_{1/2}$–$(^2D, ^3P)\ ^2D^o_{3/2}$	G	77.340	35	67.569	30	59.612	20	53.044	10
$4p\ ^2P^o_{3/2}$–$(^2D, ^1D)\ ^2P_{3/2}$	t					59.826	2		
$4p\ ^2P^o_{3/2}$–$(^2D, ^1D)\ ^2S_{1/2}$	u	77.436	5*l*						
$4s\ ^2S_{1/2}$–$(^2D, ^3P)\ ^4P^o_{1/2}$	H	77.667	5	67.768	5	59.722	5	53.095	3
$4s\ ^2S_{1/2}$–$(^2D, ^3P)\ ^4F^o_{3/2}$	I	77.910	5*w*	68.022	2	59.971	5	53.335	3
$4s\ ^2S_{1/2}$–$(^2D, ^3P)\ ^4P^o_{3/2}$	J	78.424	25	68.476	15	60.383	10	53.725	5

[a] Levels are designated in *LS* coupling: The parent terms for $3d^9$ and for the coupled external electrons $4s4p$ or $4p^2$ are given in parentheses. A code has been attributed to the transitions to facilitate correspondence with Fig. 1. Capital letters denote $3d^{10}4s$–$3d^94s4p$ transitions; lower-case letters denote $3d^{10}4p$–$3d^94p^2$ transitions. Symbols: *u*, unresolved; *w*, wide; *l*, shaded to longer wavelengths; *p*, perturbed by close line; *, doubly classified. Lines for which a question mark is given have observed intensities much larger than expected; they may be blended with lines of other ionization stages. Not all the transitions are shown in Fig. 1.

the transitions may be written as $[3d^{10}(^1S)]4s$–$[3d^94p(L,S)]4s$, the intensities are proportional to the amount of $[3d^94p(^1P)]4s\ ^2P^o_{1/2}$ state in the upper level. For the line marked *D* in Fig. 1, this is calculated as 4.9% for Mo, 3.9% for Nb, 2.5% for Zr, and 0.9% for Y. Therefore the low intensity found for this transition in Y XI is theoretically justified. Tracings of a portion of the satellite spectra observed in each element are shown in Fig. 1.

The least-squares calculation for the $3d^94s4p$ levels involves fitting the ten observed levels with the eight Slater parameters for the $3d^94s4p$ configuration: A, $F^2(3d4p)$, $G^1(3d4p)$, $G^3(3d4p)$, $G^1(4s4p)$, $G^2(3d4s)$, ζ_{3d}, and ζ_{4p}. As $G^3(3d4p)$ has a constant contribution to the terms having $J = 1/2, 3/2$ levels ($^{2,4}P$, $^{2,4}D$, ^4F), its value could be fixed at the HF value, leaving seven parameters to be varied.

By optimizing the remaining seven parameters, we could obtain good agreement between calculated and observed energies. Also, the resultant scaling factors for the HF parameters of the four ions were found to be quite similar. Nevertheless, their variation along the sequence was not completely regular. The irregularities are undoubtedly due to small perturbations that may be expected for such high configurations. For example, the $3d^107p$ configuration overlaps $3d^94s4p$ and, as the relative position of the two configurations varies along the sequence, different repulsion effects may be expected. As the ratio of observed levels to free parameters is small, the parameter values are thus sensitive to such small perturbations.

In order to reduce the number of free parameters and improve their reliability, we adopted a generalized least-squares (GLS) procedure in which the four observed spectra were treated simultaneously. In this procedure the HF values of the integrals were entered explicitly into the energy matrices as coefficients of the angular factors and the scaling factors for the HF parameters considered as free parameters. The scaling factors $SF(Z)$ were constrained to be linearly dependent on Z: $SF(Z) = SF_{av} + a(Z - Z_{av})$. (For the present ions, $Z_{av} = 40.5$.) However, with this constraint, the coefficient a of the linear term in the GLS procedure was undefined for all parameters except $G^1(4s4p)$ and ζ_{3d}. We thus set $a = 0$ except for these two parameters, leaving 13 parameters to account for the 40 observed levels. The resultant root-mean-square deviation of this fit, 122 cm^{-1}, is comparable with the uncertainty of the energy-level values, which is about

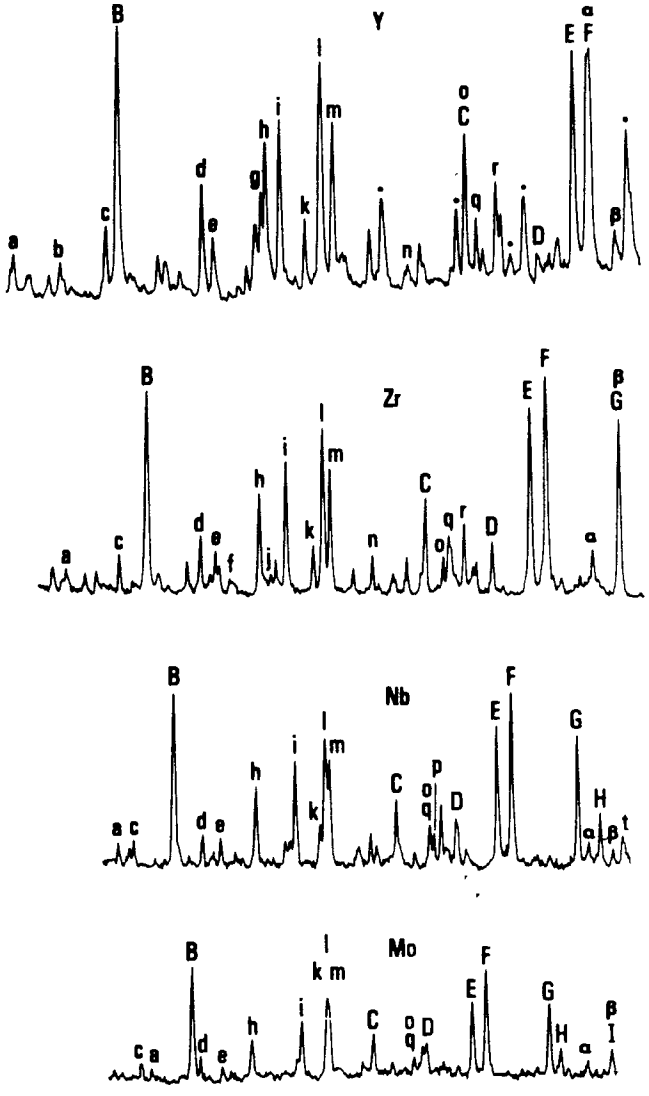

Fig. 1. Comparison of the spectra of Y XI, Zr XII, Nb XIII, and Mo XIV showing isoelectronic regularities in the region of the strongest $3d^{10}4s$–$3d^{9}4s4p$ transitions (capital letters), $3d^{10}4p$–$3d^{9}4p^2$ transitions (lower-case letters), and $3d^{10}4s$–$3d^{10}7p$ transitions (Greek letters). Complete designations are given in Tables 1 and 7. Lines marked with dots pertain to higher ionization stages in Y; two of them have been classified as Y XIV.[6]

140 cm^{-1}. Compared with the independent calculations, the GLS process does not produce changes in any of the line identifications. Only nine lines have deviations $\Delta\sigma = \sigma_{exp} - \sigma_{calc}$ larger than the experimental uncertainty.

The $3d^{9}4s4p$ energy levels are listed in Table 2. The levels are designated in the $3d^{9}(^2D)4s4p(^{1,3}P^{\circ})$ SLJ scheme, which proved to be the best of the several possible schemes.

The fitted values of the scaling factors and parameter values are given in Tables 3 and 4, respectively. In Table 5 we list the HF values of the parameters.

$3d^{10}4p$–$3d^{9}4p^2$ Transitions

With the strongest satellite lines accounted for by the $3d^{10}4s$–$3d^{9}4s4p$ transitions, we then tried to correlate the remaining lines with the group expected to be next in strength, $3d^{10}4p$–$3d^{9}4p^2$. When we did this, application of the GLS procedures used for the $3d^{9}4s4p$ configurations proved to be important.

The $3d^{9}4p^2$ configuration is expected to lie below the ionization limit in the present ions. It has a total of 28 levels, of which 21 have J = 1/2, 3/2, 5/2 and can combine with $4p\ ^2P^{\circ}_{1/2,3/2}$. Because of strong electrostatic interactions within the n = 4 shell, the $3d^{9}4p^2$ configuration is expected to be perturbed by the $3d^{9}4s^2$, $3d^{9}4s4d$, and $3d^{9}4d^2$ configurations, which do not radiate to the $3d^{10}nl$ levels. They show their presence mainly by perturbing the $3d^{9}4p^2$ levels. The $3d^{9}4s^2$ and $3d^{9}4d^2$ configurations are expected to be far enough from $3d^{9}4p^2$ that their perturbations can be treated by effective electrostatic interactions. However, $3d^{9}4s4d$ is close to $3d^{9}4p^2$ and must be specifically included in the energy matrix. Our matrix thus included the 18 ordinary electrostatic and spin–orbit parameters for these two interacting configurations plus a correction of the type $\alpha L(L+1)$ for the terms of the subconfiguration $4p^2$ and a similar one for the final terms of $3d^{9}4p^2$.

From an initial set of scaled HF parameters, predicted wavelengths and line strengths for the $3d^{10}4p$–$3d^{9}4p^2$ transitions could be calculated. This led to the identification of several strong lines of this array and also made it evident that the levels of $3d^{9}4s4d$ and about 10 levels of $3d^{9}4p^2$ would not be observable with the present data. Ensuing least-squares calculations were made by fixing the internal $3d^{9}4s4d$ parameters at their HF values. The position of the $3d^{9}4s4d$ configuration relative to $3d^{9}4p^2$ was fixed in such a way that the separation between their lowest levels would equal the value of $E(3d^{10}4d)$–$2E(3d^{10}4p)$ as given by the known levels of the one-electron system. Thus all $3d^{9}4s4d$ parameters were fixed except the $3d^{9}4s4d$–$3d^{9}4p^2$ configuration interaction integral $R^1(4p4p, 4s4d)$. Again, a GLS procedure was used for fitting the $3d^{9}4p^2$ parameters and $R^1(4p4p, 4s4d)$. The scaling factors of $F^2(3d4p)$, $G^1(3d4p)$, $G^3(3d4p)$, ζ_{3d}, and $R^1(4p4p, 4s4d)$ were assumed to be constant along the sequence. Scaling factors for $F^2(4p4p)$ and ζ_{4p} were left unconstrained.

By reducing the number of free parameters to 17, and carrying out successive line identifications and least-squares calculations, we could obtain values for 44 $3d^{9}4p^2$ energy levels in the four ions. The fitted and HF values of the parameters for the $3d^{9}4p^2$ configurations are given in Tables 4 and 5, respectively. Table 5 also includes the HF values for $3d^{9}4s4d$. In the least-squares fits to the observed levels, the $\alpha L(L+1)$ correction for the final terms of $3d^{9}4p^2$ remained undefined and was dropped. The fitted values of α for the terms of $4p^2$ are given in Table 4. The final root-mean-square deviation of the calculated values was 200 cm^{-1}.

The identified $3d^{10}4p$–$3d^{9}4p^2$ transitions are given in Table 1. The $3d^{9}4p^2$ energy levels are given in Table 6. For designating the levels, no entirely satisfactory coupling scheme could be found. We have adopted the $(3d^9\ S_1L_1, 4p^2\ S_2L_2)$ SLJ scheme, although it is not appreciably better than the $(3d^9\ S_1L_1J_1, 4p^2\ S_2L_2J_2)$ J scheme. The lack of a pure coupling scheme results from the presence of electrostatic and spin–orbit terms of comparable magnitude in the Hamiltonian. The labeling of levels is further complicated by the changing importance of these interactions along the sequence. For example, the ratio $F^2(4p4p)/\zeta_{4p}$ decreases from 5.5 in Y XI to 3.5 in Mo XIV. Therefore significant changes occur

Table 2. Experimental Energy Levels of the $3d^9 4s4p$ Configurations of Y XI, Zr XII, Nb XIII, and Mo XIV[a]

		Y XI			Zr XII			Nb XIII			Mo XIV		
J	Designation	E (cm^{-1})	ΔE	Percent	E (cm^{-1})	ΔE	Percent	E (cm^{-1})	ΔE	Percent	E (cm^{-1})	ΔE	Percent
1/2	$(^2D, ^3P)\ ^4P^\circ$	1 287 540	−20	81	1 475 630	−120	77	1 674 440	50	73	1 883 400	−50	68
	$(^2D, ^3P)\ ^2P^\circ$	1 301 350	50	90	1 489 840	10	85	1 688 800	60	82	1 898 000	0	79
	$(^2D, ^3P)\ ^4D^\circ$	1 304 450	*[b]	79	1 494 150	90	71	1 694 450	20	63	1 905 750	140	56
	$(^2D, ^1P)\ ^2P^\circ$	1 357 980	−90	98	1 551 210	260	97	1 754 350	−170	97	1 968 960	130	96
3/2	$(^2D, ^3P)\ ^4P^\circ$	1 275 120	70	64	1 460 370	−80	58	1 656 110	230	52	1 861 340	90	46
	$(^2D, ^3P)\ ^4F^\circ$	1 283 530	60	86	1 470 100	−200	85	1 667 480	−10	84	1 874 940	−60	84
	$(^2D, ^3P)\ ^2D^\circ$	1 292 990	−30	54	1 479 960	−100	53	1 677 520	50	52	1 885 220	−50	50
	$(^2D, ^3P)\ ^2P^\circ$	1 300 060	150	59	1 488 080	−40	58	1 686 760	20	57	1 895 720	−60	57
	$(^2D, ^3P)\ ^4D^\circ$	1 311 070	50	52	1 501 560	20	52	1 702 750	−60	52	1 914 770	−90	51
	$(^2D, ^1P)\ ^2P^\circ$	1 343 080	−80	92	1 533 750	160	91	1 734 240	−180	90	1 945 620	−50	89
	$(^2D, ^1P)\ ^2D^\circ$	[1 372 610]		96	[1 566 430]		96	[1 770 900]		95	[1 986 080]		94

[a] The deviations $\Delta E = E_{exp} - E_{th}$ are taken from the generalized least-squares treatment of the whole sequence. The percentage of the leading LS component is given. Predicted energies for the $(^2D, ^1P)\ ^2D^\circ_{3/2}$ levels are given in brackets.
[b] *Level value based on eyepiece measurement; not used in least-squares fit.

Table 3. Fitted Scaling Factors for the Hartree–Fock Integrals

Parameter	Y XI	Zr XII	Nb XIII	Mo XIV	Footnotes
$F^2(4p4p)$	0.772 ± 0.014	0.769 ± 0.013	0.733 ± 0.013	0.720 ± 0.013	[a]
$F^2(3d4p)$	0.987 ± 0.007	0.987	0.987	0.987	[a,1]
	0.992 ± 0.006	0.992	0.992	0.992	[b,1]
$G^1(3d4p)$	0.983 ± 0.008	0.983	0.983	0.983	[a,1]
	0.981 ± 0.007	0.981	0.981	0.981	[b,1]
$G^3(3d4p)$	0.983	0.983	0.983	0.983	[a,2]
$G^2(3d4s)$	1.012 ± 0.018	1.012	1.012	1.012	[b,1]
$G^1(4s4p)$	0.786 ± 0.001	0.789 ± 0.001	0.791	0.794	[b,3]
ζ_{3d}	1.049 ± 0.012	1.049	1.049	1.049	[a,1]
	1.028 ± 0.006	1.024 ± 0.006	1.021	1.018	[b,3]
ζ_{4p}	1.090 ± 0.012	1.088 ± 0.008	1.094 ± 0.007	1.095 ± 0.007	[a]
	1.120 ± 0.005	1.125	1.125	1.125	[b,1]
$R^1(4p4p, 4s4d)$	0.956 ± 0.066	0.956	0.956	0.956	[a,1]

[a] GLS fit of $3d^9 4p^2 + 3d^9 4s4d$.
[b] GLS fit of $3d^9 4s4p$.
[1] An equal value has been assumed for the four elements.
[2] The same scaling factor has been assumed for $G^3(3d4p)$ and $G^1(3d4p)$.
[3] The scaling factors are constrained to be linearly dependent on the atomic number.

in the eigenvectors, as is seen in Table 6, and also in some of the calculated line strengths. Our names for levels having leading percentages of less than 50% are assigned mainly for use with the classified line list.

Identification of the $3d^{10}7p\ ^2P^\circ$ Term

Comparison of the spectra in Fig. 1 shows that in Y XI line F is weaker relative to the other $3d^{10}4s$–$3d^9 4s4p$ transitions and is split into two components. The two components (76.920 and 76.928 Å) both have the excitation character of Y XI. If these lines are taken as transitions to the ground state, they would involve upper levels with effective quantum numbers $n^* = 6.0737$ and $n^* = 6.0725$, respectively. As the known members of the $3d^{10}np\ ^2P^\circ_{3/2}$ series have effective quantum numbers $n^*(4p) = 3.0245$, $n^*(5p) = 4.0546$, and $n^*(6p) = 5.0667$, there is little doubt that one of these lines is $4s\ ^2S_{1/2}$–$7p\ ^2P^\circ_{3/2}$. If we identify a line at 77.058 Å as $4s\ ^2S_{1/2}$–$7p\ ^2P^\circ_{1/2}$, we obtain a value of $\delta n^* = n^*(j = 3/2) - n^*(j = 1/2)$ of 0.0196 if 76.920 Å is identified as $4s\ ^2S_{1/2}$–$7p\ ^2P^\circ_{3/2}$ and 0.0184 if 76.928 Å is used for this transition. Because of the regularity of δn^* for the lower members of the np series (0.0192 for $4p$, 0.0188 for $5p$, and 0.0187 for $6p$), we consider 76.928 Å as the best choice for $4s\ ^2S_{1/2}$–$7p\ ^2P^\circ_{3/2}$. The reduced intensity of F in Y XI is undoubtedly caused by mixing between the $3d^9(^2D)4s4p(^3P)\ ^2P^\circ_{3/2}$ and $3d^{10}7p\ ^2P^\circ_{3/2}$ states, which makes unambiguous identification of the two lines difficult.

In Mo XIV Curtis *et al.*[8] classified lines at 53.19 ± 0.05 Å and 53.30 ± 0.05 Å as $4s\ ^2S_{1/2}$–$7p\ ^2P^\circ_{3/2}$ and $4s\ ^2S_{1/2}$–$7p\ ^2P^\circ_{1/2}$ transitions, respectively. These wavelengths agree with our present values for these lines, 53.221 ± 0.005 Å and 53.335 ± 0.005 Å. However, it is clear from isoelectronic considerations that most of the intensity of the 53.335-Å line is due to the $3d^{10}4s\ ^2S_{1/2}$–$3d^9(^2D)4s4p(^3P)\ ^4F^\circ_{3/2}$ transition. Our new value for the $7p\ ^2P^\circ_{3/2}$ level, 1 878 940 cm^{-1}, is confirmed by observation of the $4d\ ^2D_{5/2}$–$7p\ ^2P^\circ_{3/2}$ transition at 87.717 Å.

Our wavelengths for the $4s$–$7p$ transitions in Y XI, Zr XII, Nb XIII, and Mo XIV are given in Table 7. The lines are noted

Table 4. Fitted Parameter Values (in cm^{-1}) for the $3d^9 4s4p$ and $3d^9 4p^2$ Configurations of Y XI, Zr XII, Nb XIII, and Mo XIV

Configuration	Parameter	Y XI	Zr XII	Nb XIII	Mo XIV
$3d^9 4s4p$	A	1 339 595	1 529 988	1 730 788	1 241 997
	$G^2(3d4s)$	19 422	20 452	21 479	22 501
	$F^2(3d4p)$	53 883	57 598	61 268	64 899
	$G^1(3d4p)$	17 428	18 610	19 779	20 935
	$G^3(3d4p)$	17 362[a]	18 605[a]	19 832[a]	21 046[a]
	$G^1(4s4p)$	93 059	98 402	103 703	108 974
	ζ_{3d}	6 959	8 103	9 376	10 787
	ζ_{4p}	13 128	15 770	18 741	22 068
$3d^9 4p^2$	A	1 565 492	1 774 993	1 994 607	2 225 502
	$F^2(3d4p)$	53 462	57 155	60 803	64 413
	$G^1(3d4p)$	17 404	18 590	19 763	20 924
	$G^3(3d4p)$	17 013	18 236	19 444	20 639
	$F^2(4p4p)$	69 351	72 864	73 041	75 265
	$\alpha(4p4p)$	−1 017	−1 017	−1 017	−1 017
	ζ_{3d}	7 107	8 302	9 638	11 125
	ζ_{4p}	12 684	15 214	18 184	21 435
Configuration Interaction	$R^1(4p4p, 4s4d)$	105 857	112 338	118 640	124 790

[a] Fixed at HF value.

Table 5. Hartree–Fock Integrals (in cm^{-1}) for the configurations $3d^9 4s4p$, $3d^9 4p^2$, and $3d^9 4s4d$ of Y XI, Zr XII, Nb XIII, and Mo XIV

Configuration	Integral	Y XI	Zr XII	Nb XIII	Mo XIV
$3d^9 4s4p$	E_{av}	1 326 636	1 519 359	1 724 419	1 937 001
	$G^2(3d4s)$	19 184	20 202	21 216	22 226
	$F^2(3d4p)$	54 307	58 052	61 751	65 410
	$G^1(3d4p)$	17 764	18 969	20 160	21 339
	$G^3(3d4p)$	17 362	18 605	19 832	21 046
	$G^1(4s4p)$	118 392	124 758	131 028	137 217
	ζ_{3d}	6 770	7 909	9 183	10 600
	ζ_{4p}	11 668	14 015	16 657	19 613
$3d^9 4p^2$	E_{av}	1 525 782	1 733 589	1 953 431	2 181 418
	$F^2(3d4p)$	54 193	57 937	61 635	65 294
	$G^1(3d4p)$	17 698	18 904	20 097	21 277
	$G^3(3d4p)$	17 300	18 544	19 772	20 987
	$F^2(4p4p)$	89 810	94 775	99 675	104 519
	ζ_{3d}	6 772	7 911	9 184	10 601
	ζ_{4p}	11 640	13 985	16 624	19 579
$3d^9 4s4d$	E_{av}	1 643 121	1 862 502	2 093 871	2 332 554
	$F^2(3d4d)$	46 395	50 995	55 546	60 053
	$F^4(3d4d)$	21 681	24 038	26 379	28 705
	$G^0(3d4d)$	15 728	17 215	18 673	20 105
	$G^2(3d4d)$	18 298	20 210	22 099	23 966
	$G^4(3d4d)$	13 497	15 457	16 954	18 438
	$G^2(3d4s)$	19 224	20 230	21 234	22 235
	$G^2(4s4d)$	80 820	86 671	92 274	97 663
	ζ_{3d}	6 780	7 920	9 193	10 610
	ζ_{4d}	1 147	1 435	1 766	2 146
Configuration Interaction	$R^1(4p4p, 4s4d)$	110 744	117 524	124 116	130 550

as α and β in Fig. 1. The $7p$ energy levels are given in Table 8.

$3d$–$4p$ Transitions in Zn-like and Ni-like Ions

The remaining satellite lines are the $3d^{10}4s^2$–$3d^9 4s^2 4p$ transitions in the Zn-like ions. Our identifications for the $3d^9 4s^2 4p\ {}^1P_1^\circ$ and ${}^3D_1^\circ$ levels of Y X, Zr XI, and Nb XII are given in Table 9. Our new measurements for these transitions in Mo XIII are also given here. The $3d^{10}4s^2\ {}^1S_0$–$3d^9 4s^2 4p\ {}^3P_1^\circ$ transition, expected to be weak, has not been observed.

Our measurements for the $3d^{10}$–$3d^9 4p$ resonance lines of the Ni-like ions Y XII, Zr XIII, Nb XIV, and Mo XV are given in

Table 6. Experimental Levels of $3d^9 4p^2$ [a]

		Y XI			Zr XII			Nb XIII			Mo XIV		
J	Designation	E (cm^{-1})	ΔE	Percent	E (cm^{-1})	ΔE	Percent	E (cm^{-1})	ΔE	Percent	E (cm^{-1})	ΔE	Percent
1/2	$(^2D, {}^1D)\ {}^2S$	1 499 890	150	57	1 704 070	−160	57	1 918 750	180	59	2 143 950	40	59
	$(^2D, {}^3P)\ {}^4D$	1 506 550	−160	79	1 712 880	0	79	[1 929 750]		81	[2 157 680]		81
	$(^2D, {}^1D)\ {}^2P$	1 516 750?		62	1 724 700?		62	[1 942 150]		62	[2 171 190]		62
	$(^2D, {}^3P)\ {}^2P$	1 534 050	100	86	1 742 110	160	86	1 960 760	−10	87	2 190 700	80	88
	$(^2D, {}^3P)\ {}^4P$	[1 541 140]		83	1 751 810	−30	81	[1 973 850]		80	[2 207 330]		78
3/2	$(^2D, {}^3P)\ {}^4D$	1 495 570?		69	1 699 310	70	67	[1 913 240]		64	[2 137 880]		62
	$(^2D, {}^1D)\ {}^2P$	1 500 720?		66	1 704 740?		65	1 918 760?		64	2 143 940?		63
	$(^2D, {}^3P)\ {}^2D$	1 512 840	−60	42[b]	1 717 720	−20	46	1 932 740	70	49	2 158 460	270	51
	$(^2D, {}^3P)\ {}^4F$	1 519 020	50	36[c]	1 725 880	40	40	1 943 180	−320	44	2 171 600	−500	46
	$(^2D, {}^1D)\ {}^2D$	1 524 990	−40	56	1 732 710	−20	55	1 950 830	−30	55	2 180 320	0	54
	$(^2D, {}^3P)\ {}^2P$	1 536 320	−120	24[d]	1 745 170	−150	57	1 964 340	−170	61	2 194 630	−120	62
	$(^2D, {}^3P)\ {}^4P$	1 538 060	270	31[e]	[1 747 680]		46	1 969 260	160	45	[2 202 130]		43
	$(^2D, {}^1S)\ {}^2D$	[1 577 960]		86	[1 790 120]		84	[2 011 970]		82	[2 246 300]		80
5/2	$(^2D, {}^3P)\ {}^4D$	[1 484 890]		52	[1 685 980]		48	[1 896 670]		45	[2 117 650]		42
	$(^2D, {}^3P)\ {}^2F$	[1 503 800]		53	[1 707 860]		53	[1 922 230]		51	[2 147 280]		50
	$(^2D, {}^3P)\ {}^4P$	[1 506 180]		38	[1 710 790]		41	[1 925 540]		43	[2 151 050]		45
	$(^2D, {}^3P)\ {}^4F$	[1 520 030]		28[f]	1 727 180	150	32	1 944 890	110	35	[2 173 560]		39
	$(^2D, {}^1D)\ {}^2F$	[1 522 800]		23[g]	[1 730 340]		25[h]	[1 948 520]		28	[2 177 840]		31
	$(^2D, {}^3P)\ {}^2D$	1 532 560	−50	54	1 740 950	−40	53	1 960 070	140	52	2 190 210	110	51
	$(^2D, {}^1D)\ {}^2F$	1 542 590	−100	58	1 753 410	−20	56	1 974 930	60	51	2 208 210	380	47
	$(^2D, {}^1S)\ {}^2D$	1 561 470	40	83	1 770 980	110	80	1 989 710	−100	76	2 220 830	−160	71

[a] The deviations $\Delta E = E_{exp} - E_{th}$ are taken from the generalized least-squares treatment of the whole sequence. Predicted energies for unknown levels are given in brackets. The designations are given in LS coupling with parent term of $4p^2$ in parentheses. The percentages of the leading eigenvector components are also given.

[b] Leading component, $(^3P)\ {}^4F$, 49%.
[c] Leading component, $(^3P)\ {}^2D$, 40%.
[d] Leading component, $(^1D)\ {}^2P$, 26%.
[e] Leading component, $(^3P)\ {}^2P$, 47%.
[f] Leading component, $(^3P)\ {}^4P$, 30%.
[g] Leading component, $(^3P)\ {}^4F$, 29%.
[h] Leading component, $(^3P)\ {}^4F$, 26%.

Table 7. $3d^{10}4s$–$3d^{10}7p$ Transitions in Y XI, Zr XII, Nb XIII, and Mo XIV

Transition	Code	Y XI	Zr XII	Nb XIII	Mo XIV
$3d^{10}4s\ {}^2S_{1/2}$–$3d^{10}7p\ {}^2P^o_{3/2}$	α	76.931	67.440	59.666	53.228
$3d^{10}4s\ {}^2S_{1/2}$–$3d^{10}7p\ {}^2P^o_{1/2}$	β	77.064	67.576[a]	57.793	53.341[b]

[a] Blended with $3d^{10}4s\ {}^2S_{1/2}$–$3d^9 4s4p\ (^2D, {}^3P)\ {}^2D^o_{3/2}$.
[b] Blended with $3d^{10}4s\ {}^2S_{1/2}$–$3d^9 4s4p\ (^2D, {}^3P)\ {}^4F^o_{3/2}$.

Table 8. Energy Levels (in cm^{-1}) of the $3d^{10}7p$ Configurations of Y XI, Zr XII, Nb XIII, and Mo XIV[a]

Designation	Y XI	Zr XII	Nb XIII	Mo XIV
$3d^{10}7p\ {}^2P^o_{1/2}$	1 297 620	(1 479 820)	1 672 440	(1 874 730)
$3d^{10}7p\ {}^2P^o_{3/2}$	1 299 870	1 482 800	1 676 000	1 878 710

[a] The values in parentheses are derived from blended lines.

Table 9. $3d$–$4p$ Transitions in Ni-like and Zn-like Ions

Transition	λ(Å)	Int.	λ(Å)	Int.	λ(Å)	Int.	λ(Å)	Int.
	Y XII		Zr XIII		Nb XIV		Mo XV	
$3d^{10}\ {}^1S_0$–$3d^9 4p\ {}^3D^o_1$	72.103	80	63.234	100	55.963	100	49.914	100
$^1P^o_1$	72.734	100	63.828	150	56.523	150	50.448	150
$^3P^o_1$	73.588	5	64.538	5	57.119	5	50.956	5
	Y X		Zr XI		Nb XII		Mo XIII	
$3d^{10}4s^2\ {}^1S_0$–$3d^9 4s^2 4p\ {}^3D^o_1$	78.706	10	68.562	5	60.332	10	53.551	10
$^1P^o_1$	79.338[a]	100	69.161	15	60.902	20	54.101	20

[a] Blended with $3p^6 3d^8\ {}^1G_4$–$3p^5 3d^9\ {}^1F_3$ transition of Y XIV.

Table 9. For some lines they differ significantly from the earlier values of Alexander *et al.*[9] Our assignment of the line at 73.588 Å as $3d^{10}\,{}^1S_0$–$3d^9 4p\,{}^3P_1^\circ$ in Y XII represents a revised line identification from that given in Ref. 9.

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Note added in proof: Recent measurements in second and third orders have indicated systematic shifts in our wavelenths for Zr XII and Nb XIII. The improved values for Zr XII (in Å) are as follows (intensities are in parentheses):

64.488 (20)	65.775 (10)	66.341 (2)	67.130 (30)
64.814 (1w)	65.910 (10)	66.608 (8)	67.209(50)
65.080 (2)	65.832 (1)	66.699 (3)	67.576 (30)
65.218 (50)	65.044 (5)	66.727 (5p)	67.774 (5)
65.484 (5)	66.094 (20)	66.803 (5)	68.028 (2)
65.557 (3)	66.129 (10)	66.938 (3)	68.479 (15)

The improved values for Nb XIII are:

58.367 (8)	58.893 (5)	59.295 (40)	59.984 (5)
58.391 (20)	58.917 (3)	59.623 (20)	60.397 (10)
58.413 (10)	59.024 (5w)	59.836 (2)	
58.735 (10)	59.223 (20)	59.733 (5)	

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Spectra of the cobaltlike ions Sr XII, Y XIII, Zr XIV, Nb XV, and Mo XVI

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Spectra of the cobaltlike ions Sr XII, Y XIII, Zr XIV, Nb XV, and Mo XVI have been observed by means of a low-inductance vacuum spark and a 10.7-m grazing-incidence spectrograph in the region 40–95 Å. For Y XIII, Zr XIV, Nb XV, and Mo XVI more than 40 transitions of the type $3d^9$–$3d^84p$ were identified in each ion. For Sr XII about 20 such transitions were identified. The identifications were made with the aid of Hartree–Fock and least-squares parametric calculations. New wavelengths were obtained for the $3p^63d^9$–$3p^53d^{10}$ transitions in these ions. The previous analysis of Mo XVI was partially revised and extended.

The spectra of atoms of highly ionized molybdenum have been of increased interest lately because of their use in connection with tokamak fusion research. Spectra of the cobaltlike ion Mo XVI have been observed in the TFR tokamak in France[1] as well as in the DITE tokamak in England.[2] Current studies also indicate the likely use of niobium and zirconium in future reactors. It is thus important to obtain well-established line identifications for highly ionized atoms of these elements. In the present paper we report line identifications and energy levels for the isoelectronic sequence of cobaltlike ions Sr XII, Y XIII, Zr XIV, Nb XV, and Mo XVI.

Ions of the Co I isoelectronic sequence have the ground configuration $3p^63d^9$. The first excited configuration is $3p^53d^{10}$, which gives rise to three strong resonance transitions at relatively long wavelengths (70 Å in Mo XVI). The next excited odd configuration is $3p^63d^84p$, which gives rise to a complex group of resonance lines at somewhat shorter wavelengths (45 Å in Mo XVI).

The $3p^63d^9$–$3p^53d^{10}$ transitions of Sr XII, Y XIII, Zr XIV, and Mo XVI were first observed by Edlén,[3] although no wavelength measurements were reported. Edlén's preliminary wavelengths for these ions can be inferred from the data in Table 27 of his review monograph[4]; for Sr XII, Y XIII, and Zr XIV, the wavelengths may also be inferred from the level values given in *Atomic Energy Levels*.[5] In 1971, Alexander *et al.*[6] reported measurements for the $3p^63d^9$–$3p^53d^{10}$ transitions of Y XIII–Mo XVI. New wavelengths for these transitions in Mo XVI were given in 1980 by Burkhalter *et al.*[7] Wavelengths for the same transitions in Sr XII were given recently by Acquista and Reader.[8]

The $3d^9$–$3d^84p$ transitions of Sr XII and Y XIII were first observed by Edlén. The transition groups are indicated on the spectrograms in Fig. 2 of Ref. 3 and in Fig. 49 of Ref. 4. No wavelengths were given. Alexander *et al.*[6] published wavelengths with no identifications for about 25 lines of this group in each of the ions from Y XIII to Mo XVI. Mansfield *et al.*[2] used a laser-produced plasma to observe this group in Mo XVI. They reported identifications for 25 lines. These identifications were revised and extended to a total of 38 lines by Burkhalter *et al.*[7] Our present work further revises these identifications and extends the number to 43.

EXPERIMENT

The measurements were taken from spectrograms made in connection with a recent investigation[9] of the spectra of the ironlike ions Sr XIII–Mo XVII. The spectra were made on the 10.7-m grazing-incidence spectrograph at the National Bureau of Standards (NBS). The grating had 1200 lines/mm. The angle of incidence used for Y, Zr, Nb, and Mo was 85°. This resulted in a plate factor of 0.12 Å/mm at 60 Å. The spectrum of Sr was photographed at an angle of incidence of 80°. The plate factor was 0.17 Å/mm. The spectra were excited by means of a low-inductance vacuum spark operating at a capacitance of 14 μF and a voltage of 10 kV.

One set of plates was measured with the aid of a semiautomatic comparator at the Institute for Spectroscopy in Moscow.[10] Wavelengths were calculated by using a computer code that provided an approximation of the plate-correction curve by a cubic polynomial. Secondary standards of wavelength were obtained by measurements of lines in the second order relative to impurity lines of oxygen and fluorine as well as lines of Y–Mo in various stages of ionization.[9,11–14] A second set of plates was measured at NBS. For this set all lines were measured in the second order. Averages of the wavelengths from the two sets were used for the finally adopted values.

Intensities for the observed lines of Y–Mo were derived in Moscow from densitometer recordings of the spectrograms by use of an estimated characteristic curve to represent the response of the photographic plate. For Sr XII the intensities were visually estimated from the photographic blackening. The intensity of the $3d^9\ ^2D_{5/2}$–$3d^8(^3F)4p\ ^2F_{7/2}$ transition in each spectrum was given a value of 1000.

The wavelengths, intensities, and classifications of the $3d^9$–$3d^84p$ transitions are given in Table 1. The uncertainty of the wavelengths is estimated as ±0.005 Å. The present values for the $3p^63d^9$–$3p^53d^{10}$ transitions are given in Table

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Table 1. $3d^9$–$3d^8 4p$ Transitions in Sr XII, Y XIII, Zr XIV, Nb XV, and Mo XVI

Transition	Sr XII		Y XIII		Zr XIV			Nb XV		Mo XVI	
	λ (Å)	Int.	λ (Å)	Int.	λ (Å)	Int.	Int.[a]	λ (Å)	Int.	λ (Å)	Int.
$^2D_{5/2}$–(^1S) $^2P_{3/2}$			60.662	20	53.847	90	116	48.138	80	43.324[b]	60
$^2D_{3/2}$–(^1S) $^2P_{3/2}$			61.303	10	54.437	20	33	48.685	30	43.837[b]	30
$^2D_{3/2}$–(^1S) $^2P_{1/2}$			62.111	30	55.190	100	130	49.399	160	44.509[b]	100
$^2D_{5/2}$–(^1G) $^2G_{7/2}$			63.408	90	56.141	170	177	50.091	120	45.000[b]	220
$^2D_{5/2}$–(^3P) $^2D_{3/2}$			63.964	30	56.585	110	104	50.451	110	45.290[b]	60
$^2D_{5/2}$–(^1D) $^2F_{7/2}$			64.012	60	56.597	110	44	50.435	80	45.250	30
$^2D_{5/2}$–(^3P) $^2D_{5/2}$			64.112	10	56.706	10	14				
$^2D_{3/2}$–(^3P) $^2P_{1/2}$			64.272	200	56.879	260	664	50.732	250	45.553[b]	300
$^2D_{5/2}$–(^3P) $^2P_{3/2}$	73.329	50	64.279	250	56.854	270	459	50.678	170	45.483[b]	220
$^2D_{5/2}$–(^3P) $^4D_{5/2}$			64.469	90	56.986	220	226	50.770	240	45.545	250
$^2D_{5/2}$–(^1D) $^2P_{3/2}$	73.679	150	64.555	200	57.083	290	628	50.877	400	45.659[b]	300
$^2D_{3/2}$–(^1G) $^2F_{5/2}$	73.631	250	64.569	600	57.138	700	1177	50.958	850	45.756[b]	700
$^2D_{3/2}$–(^3P) $^2S_{1/2}$			64.646	40	57.230	380[c]	200	51.055	280[c]	45.867	150
$^2D_{3/2}$–(^3P) $^2D_{3/2}$			64.677	40	57.230	380[c]	92	51.055	280[c]	45.853[b]	170
$^2D_{5/2}$–(^3P) $^4D_{7/2}$	73.772	500	64.691	600	57.241	800	659	51.038	650	45.809[b]	500
$^2D_{3/2}$–(^3P) $^2D_{5/2}$	73.932	50	64.825	200	57.360	320	340	51.155	450	45.938[b]	500
$^2D_{5/2}$–(^3P) $^4D_{3/2}$			64.851	10			17				
$^2D_{5/2}$–(^1D) $^2D_{5/2}$	74.074	150	64.906	250	57.393	290	269	51.147	200	45.887[d]	200
$^2D_{3/2}$–(^3P) $^2P_{3/2}$	74.129	100	65.003	250	57.513	450	453	51.286	700[c]	46.043[b]	1000[c]
$^2D_{5/2}$–(^1G) $^2F_{7/2}$	74.208	500	65.013	700	57.494	1000	1337	51.257	1300	46.024[b]	1600
$^2D_{5/2}$–(^1D) $^2D_{3/2}$			65.047	150	57.526	450	700	51.286	700[c]	46.043[b]	1000[c]
$^2D_{3/2}$–(^3P) $^4D_{5/2}$	74.405	100	65.194	60	57.647	180	177	51.380	220	46.113[b]	300
$^2D_{3/2}$–(^1D) $^2P_{3/2}$			65.278	20	57.748	40	136	51.490	140	46.229[b]	220
$^2D_{5/2}$–(^1D) $^2F_{5/2}$			65.304	90	57.715	260	242	51.419	400	46.131[b]	600
$^2D_{5/2}$–(^3F) $^2D_{3/2}$			65.500	40	57.851	90	120	51.516	50	46.197	110
$^2D_{5/2}$–(^3F) $^2F_{5/2}$	74.855	500	65.522	600	57.905	800	929	51.592	700	46.291[b]	650
$^2D_{3/2}$–(^3P) $^4D_{3/2}$	74.795	50	65.584	250	58.036	900[c]	671	51.763	900[c]	46.478[b]	1000[c]
$^2D_{3/2}$–(^1D) $^2D_{5/2}$			65.641	100	58.064	380	254	51.763	900[c]	46.463[b]	440
$^2D_{3/2}$–(^1D) $^2P_{1/2}$			65.667	30			2				
$^2D_{3/2}$–(^3P) $^4D_{1/2}$					58.095	190	91	51.828	140	46.573[d]	750[c]
$^2D_{5/2}$–(^3F) $^2G_{7/2}$			65.710	120	58.036	900[c]	155	51.682	300	46.352[b]	450
$^2D_{3/2}$–(^1D) $^2D_{3/2}$	75.056	250	65.785	400	58.201	500	637	51.908	400	46.623[b]	250
$^2D_{5/2}$–(^3P) $^4P_{5/2}$	75.127	500	65.823	650	58.209	1000	706	51.889	700	46.573[d]	750[c]
$^2D_{5/2}$–(^3F) $^4F_{7/2}$	75.294	250	65.847	350	58.134	500	199	51.745	350	46.378[b]	260
$^2D_{5/2}$–(^3P) $^4P_{3/2}$			65.939	10	58.284	70	19	51.935	80	46.592[d]	80
$^2D_{5/2}$–(^3F) $^4F_{5/2}$	75.427	250	65.970	150	58.247	350	158	51.849	250	46.478[b]	1000[c]
$^2D_{3/2}$–(^1D) $^2F_{5/2}$	75.400	100	66.046	40	58.395	60	77	52.045	90	46.712[b]	130
$^2D_{3/2}$–(^3F) $^2D_{3/2}$	75.687	500	66.247	250	58.534	300	255	52.145	150	46.781[b]	120
$^2D_{3/2}$–(^3F) $^2F_{5/2}$			66.271	100	58.588	180	197	52.228	1200[c]	46.877	150
$^2D_{5/2}$–(^3F) $^2D_{5/2}$	75.876	1000	66.390	1000	58.645	1000	1000	52.228	1200[c]	46.841[b]	900
$^2D_{5/2}$–(^3F) $^2F_{7/2}$	75.955	1000	66.449	1000	58.688	1000	491	52.258	1000	46.859	1000
$^2D_{3/2}$–(^3P) $^4P_{1/2}$					58.844	35	3				
$^2D_{3/2}$–(^3P) $^4P_{5/2}$			66.580	40	58.902	120	114	52.527	100	47.165[b]	170
$^2D_{3/2}$–(^3P) $^4P_{3/2}$			66.696	40	58.978	130	69	52.573	120	47.186[d]	140
$^2D_{3/2}$–(^3F) $^4F_{5/2}$	76.262	50	66.728	100	58.939	160	67	52.486	140	47.068[b]	90
$^2D_{5/2}$–(^3F) $^4F_{3/2}$			66.845	10	59.080	40	23				
$^2D_{5/2}$–(^3F) $^4G_{5/2}$			66.914	70	59.126	190	55	52.676	190	47.262[d]	180
$^2D_{5/2}$–(^3F) $^4G_{7/2}$			67.074	10	59.237	40	8	52.750	80	47.302	20
$^2D_{5/2}$–(^3F) $^4D_{5/2}$			67.234	20	59.360	50	12	52.846	110	47.382	30
$^2D_{3/2}$–(^3F) $^4D_{3/2}$			67.335	20	59.482	15	14				
$^2D_{3/2}$–(^3F) $^4F_{3/2}$			67.627	110	59.790	210	74	53.309	160	47.871[d]	150
$^2D_{3/2}$–(^3F) $^4G_{5/2}$			67.692	10	59.836	30	5				
$^2D_{5/2}$–(^3F) $^4D_{7/2}$			67.973	15	60.038	90	11	53.471	130	47.959[d]	90

[a] Calculated from fitted values of energy parameters.
[b] Present value for line given by Burkhalter *et al.*, Ref. 7.
[c] Doubly classified.
[d] Present value for line given by Burkhalter *et al.*, Ref. 7, revised classification.

2, along with the values previously reported. The present values for Sr XII are not compared with those of Ref. 8 because the measurements were taken from the same exposures and thus differ only slightly.

SPECTRUM ANALYSIS

The observations were interpreted by comparing the observed spectra with calculated wavelengths and intensities of the five

Table 2. $3p^63d^9$–$3p^53d^{10}$ Transitions in Sr XII, Y XIII, Zr XIV, Nb XV, and Mo XVI

Transition			Sr XII	Y XIII		Zr XIV		Nb XV		Mo XVI		
			λ (Å)[a]	λ (Å)[a]	λ (Å)[b]	λ (Å)[a]	λ (Å)[b]	λ (Å)[a]	λ (Å)[b]	λ (Å)[a]	λ (Å)[b]	λ (Å)[c]
$3p^63d^9$	$^2D_{3/2}$–	$3p^53d^{10}$ $^2P_{1/2}$	86.413	81.610	81.604	77.249	77.245	73.273	73.315	69.596	69.580	69.589
	$^2D_{5/2}$–	$^2P_{3/2}$	92.029	87.394	87.382	83.196	83.181	79.374	79.357	75.869	75.861	75.863
	$^2D_{3/2}$–	$^2P_{3/2}$	93.288	88.731	88.716	84.612	84.602	80.871	80.845	77.456	77.450	77.450

[a] This work.
[b] Alexander *et al.*, Ref. 6.
[c] Burkhalter *et al.*, Ref. 7.

Table 3. Energy Levels (in cm^{-1}) of Sr XII, Y XIII, Zr XIV, Nb XV, and Mo XVI[a]

Configuration	Term	J	Sr XII	Y XIII	Zr XIV	Nb XV	Mo XVI
$3p^63d^9$	^2D	5/2	0	0	0	0	0
		3/2	14 660	17 230	20 140	23 380	27 020
$3p^53d^{10}$	^2P	3/2	1 086 610	1 144 240	1 201 990	1 259 890	1 318 070
		1/2	1 171 890	1 242 570	1 314 660	1 388 140	1 463 880
$3p^63d^84p$	$(^3F)^4D$	7/2	(1 287 050)	1 471 170	1 665 610	1 870 170	2 085 110
	$(^3F)^4G$	9/2	(1 294 130)	(1 478 120)	(1 672 850)	(1 877 670)	(2 092 710)
	$(^3F)^4D$	5/2	(1 300 810)	1 487 340	1 684 640	1 892 290	2 110 510
	$(^3F)^4G$	7/2	(1 304 500)	1 490 890	1 688 130	1 895 730	2 114 080
	$(^3F)^4G$	5/2	(1 308 000)	1 494 480	1 691 340	1 898 400	2 115 860
	$(^3F)^4G$	11/2	(1 307 760)	(1 495 300)	(1 693 740)	(1 903 070)	(2 123 170)
	$(^3F)^4F$	3/2	(1 309 240)	1 495 960	1 692 640	1 899 240	2 115 970
	$(^3F)^4D$	3/2	(1 314 560)	1 502 340	1 701 320	(1 910 980)	(2 131 480)
	$(^3F)^4F$	9/2	(1 314 230)	(1 502 500)	(1 701 410)	(1 911 100)	(2 131 540)
	$(^3F)^2F$	7/2	1 316 570	1 504 910	1 703 930	1 913 580	2 134 060
	$(^3F)^4D$	1/2	(1 316 930)	(1 505 990)	(1 706 010)	(1 916 450)	(2 137 580)
	$(^3F)^2D$	5/2	1 317 940	1 506 250	1 705 180	1 914 680	2 134 880
	$(^3F)^2G$	9/2	(1 324 150)	(1 513 830)	(1 715 100)	(1 927 290)	(2 150 740)
	$(^3F)^4F$	5/2	1 325 860	1 515 840	1 716 820	1 928 660	2 151 610
	$(^3P)^4P$	3/2	(1 327 960)	1 516 560	1 715 720	1 925 490	2 146 290
	$(^3F)^4F$	7/2	1 328 130	1 518 670	1 720 160	1 932 550	2 156 190
	$(^3P)^4P$	5/2	1 331 080	1 519 200	1 717 920	1 927 180	2 147 240
	$(^3P)^4P$	1/2	(1 332 740)	(1 520 560)	1 719 550	(1 928 850)	(2 148 770)
	$(^3F)^2G$	7/2	(1 331 850)	1 521 840	1 723 070	1 934 910	2 157 400
	$(^3F)^2F$	5/2	1 335 920	1 526 200	1 726 970	1 938 290	2 160 260
	$(^3F)^2D$	3/2	1 335 890	1 526 720	1 728 560	1 941 120	2 164 640
	$(^1D)^2F$	5/2	1 340 920	1 531 320	1 732 640	1 944 800	2 167 770
	$(^1D)^2D$	3/2	1 347 000	1 537 340	1 738 330	1 949 870	2 171 880
	$(^1G)^2F$	7/2	1 347 560	1 538 150	1 739 310	1 950 950	2 172 780
	$(^1D)^2P$	1/2	(1 348 800)	1 540 060	(1 742 530)	(1 955 360)	(2 179 420)
	$(^1G)^2H$	9/2	(1 352 680)	(1 540 680)	(1 740 350)	(1 950 390)	(2 170 640)
	$(^1D)^2D$	5/2	1 350 000	1 540 680	1 742 380	1 955 150	2 179 270
	$(^3P)^4D$	1/2	(1 351 070)	(1 541 330)	1 741 460	1 952 840	2 174 190
	$(^3P)^4D$	3/2	1 351 650	1 542 000	1 743 210	1 955 260	2 178 580
	$(^3P)^4D$	7/2	1 355 530	1 545 810	1 747 000	1 959 320	2 182 980
	$(^1D)^2P$	3/2	1 357 240	1 549 100	1 751 820	1 965 510	2 190 160
	$(^3P)^4D$	5/2	1 358 660	1 551 120	1 754 830	1 969 660	2 195 620
	$(^3P)^2P$	3/2	1 363 690	1 555 670	1 758 880	1 973 240	2 198 620
	$(^3P)^2D$	5/2	1 367 250	1 559 800	1 763 500	1 978 220	2 203 870
	$(^1G)^2H$	11/2	(1 368 780)	(1 560 220)	(1 763 660)	(1 978 120)	(2 203 340)
	$(^1D)^2F$	7/2	(1 368 940)	1 562 210	1 766 880	1 982 750	2 209 940
	$(^3P)^2D$	3/2	(1 370 640)	1 563 380	1 767 250	1 982 120	2 207 940
	$(^3P)^2S$	1/2	(1 371 270)	1 564 120	1 767 480	1 982 050	2 207 240
	$(^1G)^2F$	5/2	1 372 780	1 565 960	1 770 290	1 985 780	2 212 530
	$(^3P)^4S$	3/2	(1 375 020)	(1 568 520)	(1 772 530)	(1 987 640)	(2 213 610)
	$(^3P)^2P$	1/2	(1 378 010)	1 573 120	1 778 260	1 994 520	2 222 270
	$(^1G)^2G$	7/2	(1 383 560)	1 577 090	1 781 230	1 996 370	2 222 220
	$(^1G)^2G$	9/2	(1 385 820)	(1 579 410)	(1 783 860)	(1 999 340)	(2 225 390)
	$(^1S)^2P$	1/2	(1 429 980)	1 627 250	1 832 060	2 047 710	2 273 760
	$(^1S)^2P$	3/2	(1 447 620)	1 648 480	1 857 120	2 077 400	2 308 200

[a] Values for unobserved levels, given in parentheses, are those calculated with the fitted values of the energy parameters.

ions. The calculations were made with a set of computer codes developed by the Institute of Physics of the Lithuanian Academy of Sciences.[15,16] The radial integrals were first computed by a Hartree–Fock (HF) calculation and then scaled by factors obtained by extrapolation along the Co I isoelectronic sequence.[17,18]

Although the observed spectra are complex and blended in some regions, the predicted isoelectronic trends yielded unambiguous classifications for all the identified lines. The identifications were greatly facilitated by the fact that the $3d^9$–$3d^84p$ group is well isolated from lines of other ionization

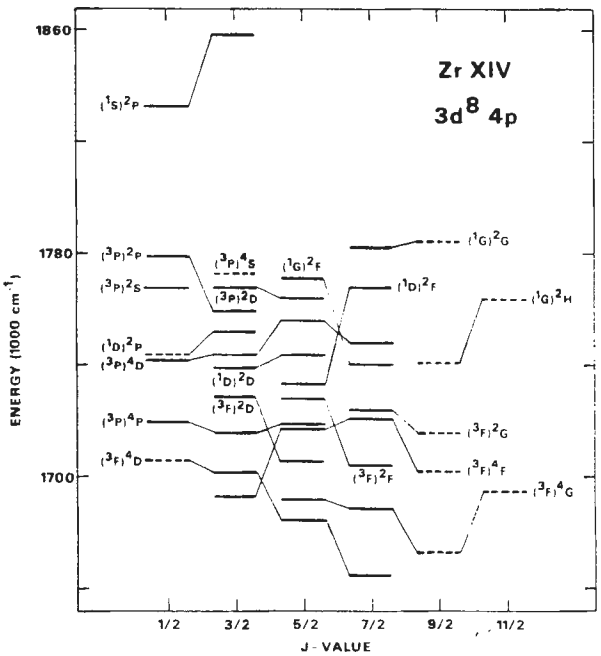

Fig. 1. Structure of the $3d^84p$ configuration of Zr XIV. The calculated positions of unobserved levels are shown as dashed lines.

Table 4. Spin–Orbit Parameters ζ_{3d} (in cm^{-1}) for the $3p^63d^9$ Configurations of Sr XII, Y XIII, Zr XIV, Nb XV, and Mo XVI

Ion	HF	Obs.	Obs./HF
Sr XII	5 836	5 864	1.005
Y XIII	6 863	6 892	1.004
Zr XIV	8 016	8 056	1.005
Nb XV	9 304	9 352	1.005
Mo XVI	10 737	10 808	1.007

Table 5. Energy Parameters (in cm^{-1}) for the $3p^53d^{10}$ Configurations of Sr XII, Y XIII, Zr XIV, Nb XV, and Mo XVI

Ion	Parameter	HF	Obs.	Obs./HF
Sr XII	E_{av}	1 100 410	1 115 040	
	ζ_{3p}	54 326	56 853	1.0465
Y XIII	E_{av}	1 155 130	1 177 020	
	ζ_{3p}	62 188	65 553	1.0541
Zr XIV	E_{av}	1 209 140	1 239 550	
	ζ_{3p}	70 877	75 113	1.0598
Nb XV	E_{av}	1 264 360	1 302 640	
	ζ_{3p}	80 448	85 500	1.0628
Mo XVI	E_{av}	1 317 920	1 366 670	
	ζ_{3p}	90 958	97 207	1.0687

Table 6. Energy Parameters and Mean Errors Δ (in cm^{-1}) for the $3d^84p$ Configurations of Sr XII, Y XIII, Zr XIV, Nb XV, and Mo XVI

Ion	Parameter	HF	Fitted	Fitted/HF
Sr XII	E_{av}	1 356 870	1 340 470 ± 130	
	$F^2(3d3d)$	214 010	192 820 ± 910	0.901 ± 0.004
	$F^4(3d3d)$	136 318	116 630 ± 3480	0.856 ± 0.026
	$\alpha_1(3d3d)$		107 ± 40	
	$F^2(3d4p)$	55 593	54 830 ± 930	0.986 ± 0.017
	$G^1(3d4p)$	18 218	17 740 ± 340	0.974 ± 0.019
	$G^3(3d4p)$	17 886	20 560 ± 2040	1.150 ± 0.114
	$\alpha(3d4p)$		69 ± 56	
	ζ_{3d}	6 088	6 180 ± 90	1.015 ± 0.015
	ζ_{4p}	11 329	12 540 ± 230	1.107 ± 0.020
	Δ		200	
Y XIII	E_{av}	1 551 260	1 530 440 ± 70	
	$F^2(3d3d)$	224 667	204 370 ± 610	0.910 ± 0.003
	$F^4(3d3d)$	143 263	130 100 ± 520	0.908 ± 0.004
	$\alpha_1(3d3d)$		71 ± 24	
	$F^2(3d4p)$	59 275	60 220 ± 530	1.016 ± 0.009
	$G^1(3d4p)$	19 399	19 210 ± 230	0.990 ± 0.012
	$G^3(3d4p)$	19 106	20 800 ± 1090	1.089 ± 0.057
	$\alpha(3d4p)$		32 ± 22	
	ζ_{3d}	7 144	7 180 ± 70	1.005 ± 0.010
	ζ_{4p}	13 586	15 150 ± 120	1.115 ± 0.009
	Δ		240	
Zr XIV	E_{av}	1 755 480	1 731 230 ± 60	
	$F^2(3d3d)$	235 264	214 890 ± 580	0.913 ± 0.002
	$F^4(3d3d)$	150 169	136 350 ± 480	0.908 ± 0.003
	$\alpha_1(3d3d)$		76 ± 24	
	$F^2(3d4p)$	62 917	63 970 ± 450	1.017 ± 0.007
	$G^1(3d4p)$	20 569	20 360 ± 220	0.990 ± 0.011
	$G^3(3d4p)$	20 312	22 150 ± 1170	1.090 ± 0.058
	$\alpha(3d4p)$		34 ± 23	
	ζ_{3d}	8 328	8 410 ± 70	1.010 ± 0.008
	ζ_{4p}	16 127	17 910 ± 110	1.111 ± 0.007
	Δ		240	
Nb XV	E_{av}	1 972 210	1 942 790 ± 70	
	$F^2(3d3d)$	245 805	226 020 ± 740	0.920 ± 0.003
	$F^4(3d3d)$	157 039	143 220 ± 610	0.912 ± 0.004
	$\alpha_1(3d3d)$		66 ± 28	
	$F^2(3d4p)$	66 526	67 860 ± 640	1.020 ± 0.010
	$G^1(3d4p)$	21 729	21 630 ± 260	0.995 ± 0.012
	$G^3(3d4p)$	21 507	22 950 ± 1490	1.067 ± 0.069
	$\alpha(3d4p)$		45 ± 27	
	ζ_{3d}	9 650	9 690 ± 70	1.004 ± 0.007
	ζ_{4p}	18 974	21 120 ± 130	1.113 ± 0.007
	Δ		270	
Mo XVI	E_{av}	2 198 910	2 165 110 ± 80	
	$F^2(3d3d)$	256 302	235 430 ± 760	0.919 ± 0.003
	$F^4(3d3d)$	163 880	149 560 ± 650	0.913 ± 0.004
	$\alpha_1(3d3d)$		51 ± 27	
	$F^2(3d4p)$	70 106	71 150 ± 660	1.015 ± 0.009
	$G^1(3d4p)$	22 879	22 810 ± 250	0.997 ± 0.011
	$G^3(3d4p)$	22 692	23 710 ± 1550	1.045 ± 0.068
	$\alpha(3d4p)$		51 ± 27	
	ζ_{3d}	11 119	11 180 ± 70	1.005 ± 0.006
	ζ_{4p}	22 150	24 690 ± 130	1.115 ± 0.006
	Δ		270	

stages. The identifications are supported by repetititon of the $3d^9\ ^2D$ fine-structure interval in the measurements. Nearly all $3d^84p$ levels with $J = 3/2$ or $J = 5/2$ have observed transitions to both of the $3d^9\ ^2D$ levels.

In general, the observed intensities compare well with the calculated values. As an example, the calculated values for Zr XIV are shown following the observed intensities in Table 1. The scale for the calculated values was obtained by setting the intensity of the $3d^9\ ^2D_{5/2}$–$3d^8(^3F)4p\ ^2D_{5/2}$ transition equal to its observed value.

The energy levels derived from the wavelength measurements are given in Table 3. The uncertainty of the values of the $3d^84p$ levels relative to the ground term is approximately $\pm 200\ cm^{-1}$. The relative values within $3d^84p$ are uncertain by about $\pm 100\ cm^{-1}$. The $3d^9\ ^2D$ intervals were derived from all observed pairs, with double weight given to the $3p^63d^9\ ^2D_{5/2,3/2}$–$3p^53d^{10}\ ^2P_{3/2}$ pair because of its longer wavelength.

The structure of the $3d^84p$ configuration of Zr XIV is shown in Fig. 1. Although the levels are designated in the LS-coupling scheme, the coupling is far from pure. In Table 3 we have given common designations to levels that derive from specific spectral lines that can be traced through the isoelectronic sequence. However, because the coupling changes along the sequence, for some levels it is not possible to adopt an LS name that corresponds to the major eigenvector com-

Table 7. Percentage Compositions for the $3d^84p$ Configurations of Sr XII, Zr XIV, and Mo XVI

J	Term	Percent J_1j	Percentage Composition (LS)
1/2	$(^3F)^4D$	73, 62, 48% ($^3F_2$, 3/2)	74, 62, 48% $(^3F)^4D$ + 19, 25, 30% $(^3P)^4D$ + 6, 8, 11% $(^1D)^2P$
	$(^3P)^4P$	62, 66, 72% ($^3P_1$, 1/2)	86, 86, 84% $(^3P)^4P$ + 5, 4, 2% $(^1D)^2P$ + 2, 3, 5% $(^3P)^4D$
	$(^3P)^4D$	61, 51, 51% ($^3P_0$, 1/2)	69, 48, 50% $(^3P)^4D$ + 12, 31, 26% $(^3F)^4D$ + 11, 0, 12% $(^1D)^2P$
	$(^1D)^2P$	42, 47, 32% ($^1D_2$, 3/2)	42, 47, 32% $(^1D)^2P$ + 32, 19, 31% $(^3P)^2P$ + 11, 2, 17% $(^3F)^4D$
	$(^3P)^2S$	66, 66, 68% ($^3P_1$, 3/2)	57, 61, 61% $(^3P)^2S$ + 27, 22, 19% $(^3P)^2P$ + 6, 7, 8% $(^3P)^4D$
	$(^3P)^2P$	60, 53, 47% ($^3P_2$, 3/2)	33, 33, 34% $(^3P)^2P$ + 32, 24, 19% $(^3P)^2S$ + 30, 35, 38% $(^1D)^2P$
	$(^1S)^2P$	93, 91, 88% ($^1S_0$, 1/2)	93, 91, 88% $(^1S)^2P$ + 3, 3, 4% $(^1D)^2P$ + 2, 3, 4% $(^3P)^4D$
3/2	$(^3F)^4F$	60, 55, 42% ($^3F_2$, 1/2)	27, 26, 20% $(^3F)^4F$ + 37, 14, 6% $(^3F)^4D$ + 10, 21, 26% $(^1D)^2D$
	$(^3F)^4D$	35, 39, 31% ($^3F_3$, 3/2)	40, 54, 50% $(^3F)^4D$ + 13, 20, 24% $(^3P)^4D$ + 7, 10, 13% $(^3P)^4P$
	$(^3P)^4P$	38, 38, 30% ($^3P_2$, 1/2)	39, 40, 33% $(^3P)^4P$ + 33, 25, 19% $(^3F)^4F$ + 14, 9, 7% $(^1D)^2P$
	$(^3F)^2D$	34, 35, 23% ($^3F_2$, 3/2)	37, 27, 16% $(^3F)^2D$ + 31, 41, 40% $(^3F)^4F$ + 23, 15, 14% $(^3P)^4P$
	$(^1D)^2D$	31, 13, 2% ($^1D_2$, 1/2)	31, 20, 11% $(^1D)^2D$ + 29, 22, 15% $(^3F)^2D$ + 12, 22, 28% $(^3P)^2P$
	$(^3P)^4D$	66, 37, 17% ($^3P_1$, 1/2)	50, 29, 14% $(^3P)^4D$ + 6, 20, 36% $(^3F)^2D$ + 6, 15, 21% $(^1D)^2D$
	$(^1D)^2P$	75, 57, 35% ($^1D_2$, 3/2)	61, 53, 38% $(^1D)^2P$ + 19, 11, 5% $(^1D)^2D$ + 3, 9, 17% $(^3P)^2P$
	$(^3P)^2P$	48, 34, 17% ($^3P_2$, 3/2)	65, 52, 37% $(^3P)^2P$ + 10, 16, 17% $(^1D)^2D$ + 10, 13, 15% $(^3P)^4D$
	$(^3P)^2D$	50, 45, 33% ($^3P_0$, 3/2)	78, 74, 69% $(^3P)^2D$ + 12, 12, 9% $(^3P)^4D$ + 3, 4, 5% $(^1S)^2P$
	$(^3P)^4S$	47, 47, 47% ($^3P_1$, 3/2)	87, 82, 75% $(^3P)^4S$ + 4, 5, 8% $(^3P)^2P$ + 3, 4, 3% $(^3P)^4P$
	$(^1S)^2P$	95, 93, 91% ($^1S_0$, 3/2)	95, 93, 91% $(^1S)^2P$ + 2, 2, 2% $(^1D)^2P$ + 1, 2, 2% $(^3P)^2D$
5/2	$(^3F)^4D$	59, 60, 56% ($^3F_3$, 1/2)	72, 66, 60% $(^3F)^4D$ + 17, 19, 18% $(^3F)^4F$ + 7, 8, 9% $(^3P)^4D$
	$(^3F)^4G$	62, 55, 43% ($^3F_2$, 1/2)	64, 56, 46% $(^3F)^4G$ + 11, 15, 19% $(^1D)^2F$ + 9, 9, 12% $(^3F)^4F$
	$(^3F)^2D$	30, 29, 25% ($^3F_4$, 3/2)	48, 46, 41% $(^3F)^2D$ + 18, 22, 26% $(^3F)^4G$ + 16, 11, 7% $(^3F)^4F$
	$(^3F)^4F$	65, 69, 66% ($^3F_3$, 3/2)	37, 35, 33% $(^3F)^4F$ + 21, 19, 16% $(^3F)^2F$ + 14, 19, 19% $(^3F)^4D$
	$(^3P)^4P$	28, 31, 29% ($^3P_2$, 1/2)	31, 27, 20% $(^3P)^4P$ + 22, 29, 32% $(^3F)^2D$ + 14, 11, 10% $(^1D)^2F$
	$(^3F)^2F$	48, 33, 21% ($^3F_2$, 3/2)	54, 43, 36% $(^3F)^2F$ + 15, 17, 15% $(^1D)^2F$ + 6, 13, 18% $(^1D)^2D$
	$(^1D)^2F$	31, 31, 34% ($^1D_2$, 1/2)	35, 26, 22% $(^1D)^2F$ + 45, 38, 28% $(^3P)^4P$ + 8, 11, 13% $(^3F)^4G$
	$(^1D)^2D$	9, 17, 25% ($^3P_2$, 3/2)	36, 21, 9% $(^1D)^2D$ + 29, 29, 24% $(^3P)^2D$ + 11, 18, 26% $(^3F)^2F$
	$(^3P)^4D$	32, 33, 28% ($^1D_2$, 3/2)	24, 17, 14% $(^3P)^4D$ + 23, 27, 24% $(^1D)^2D$ + 14, 22, 30% $(^1G)^2F$
	$(^3P)^2D$	55, 56, 57% ($^3P_1$, 3/2)	46, 40, 36% $(^3P)^2D$ + 36, 38, 40% $(^3P)^4D$ + 13, 16, 18% $(^1G)^2F$
	$(^1G)^2F$	63, 53, 43% ($^1G_4$, 3/2)	63, 53, 43% $(^1G)^2F$ + 7, 11, 16% $(^1D)^2D$ + 10, 11, 11% $(^1D)^2F$
7/2	$(^3F)^4D$	87, 89, 91% ($^3F_4$, 1/2)	77, 73, 69% $(^3F)^4D$ + 13, 15, 16% $(^3F)^4F$ + 5, 6, 8% $(^3F)^2F$
	$(^3F)^4G$	87, 89, 91% ($^3F_3$, 1/2)	68, 66, 65% $(^3F)^4G$ + 13, 14, 15% $(^3F)^2G$ + 14, 12, 12% $(^3F)^4F$
	$(^3F)^2F$	67, 74, 79% ($^3F_4$, 3/2)	53, 57, 59% $(^3F)^2F$ + 25, 20, 15% $(^3F)^4F$ + 12, 15, 18% $(^3F)^4D$
	$(^3F)^4F$	79, 86, 90% ($^3F_3$, 3/2)	47, 52, 53% $(^3F)^4F$ + 36, 28, 22% $(^3F)^2F$ + 6, 9, 14% $(^3F)^2G$
	$(^3F)^2G$	68, 61, 50% ($^3F_2$, 3/2)	64, 52, 36% $(^3F)^2G$ + 20, 28, 37% $(^1D)^2F$ + 12, 13, 12% $(^3F)^4G$
	$(^1G)^2F$	29, 49, 69% ($^1G_4$, 1/2)	32, 50, 64% $(^1G)^2F$ + 32, 14, 2% $(^1D)^2F$ + 13, 15, 14% $(^3F)^2G$
	$(^3P)^4D$	44, 51, 56% ($^3P_2$, 3/2)	44, 51, 56% $(^3P)^4D$ + 43, 26, 8% $(^1G)^2F$ + 1, 5, 14% $(^3F)^2G$
	$(^1D)^2F$	43, 47, 48% ($^1D_2$, 3/2)	43, 48, 48% $(^1D)^2F$ + 35, 33, 30% $(^3P)^4D$ + 10, 4, 1% $(^1G)^2F$
	$(^1G)^2G$	86, 88, 88% ($^1G_4$, 3/2)	88, 83, 77% $(^1G)^2G$ + 11, 14, 17% $(^1G)^2F$ + 1, 2, 3% $(^1D)^2F$
9/2	$(^3F)^4G$	97, 98, 98% ($^3F_4$, 1/2)	42, 40, 37% $(^3F)^4G$ + 33, 36, 37% $(^3F)^2G$ + 24, 23, 23% $(^3F)^4F$
	$(^3F)^4F$	97, 98, 98% ($^3F_4$, 3/2)	71, 71, 70% $(^3F)^4F$ + 23, 25, 26% $(^3F)^2G$ + 5, 3, 2% $(^3F)^4G$
	$(^3F)^2G$	96, 98, 99% ($^3F_3$, 3/2)	43, 37, 34% $(^3F)^2G$ + 53, 57, 60% $(^3F)^4G$ + 4, 5, 6% $(^3F)^4F$
	$(^1G)^2H$	92, 93, 94% ($^1G_4$, 1/2)	92, 90, 87% $(^1G)^2H$ + 7, 9, 10% $(^1G)^2G$ + 1, 1, 2% $(^3F)^2G$
	$(^1G)^2G$	92, 93, 94% ($^1G_4$, 3/2)	92, 90, 88% $(^1G)^2G$ + 7, 8, 10% $(^1G)^2H$ + 1, 1, 1% $(^3F)^4F$
11/2	$(^3F)^4G$	99, 99, 98% ($^3F_4$, 3/2)	99, 99, 98% $(^3F)^4G$ + 1, 1, 2% $(^1G)^2H$
	$(^1G)^2H$	99, 99, 98% ($^1G_4$, 3/2)	99, 99, 98% $(^1G)^2H$ + 1, 1, 2% $(^3F)^4G$

Table 8. Percentage Composition of the Levels Designated as $3d^8(^1D)4p\ ^2P_{1/2}$ and $3d^8(^3P)4p\ ^4D_{1/2}$ in Sr XII, Y XIII, Zr XIV, Nb XV, and Mo XVI

Level Designation	Percentage Composition
$(^1D)^2P_{1/2}$	42, 19, 47, 40, 32% $(^1D)^2P$ + 31, 36, 19, 28, 31% $(^3P)^2P$ + 11, 23, 2, 10, 17% $(^3F)^4D$ + 1, 13, 13, 3, 1% $(^3P)^4D$ + 5, 2, 11, 10, 11% $(^3P)^2S$ + 3, 4, 1, 2, 2% $(^1S)^2P$ + 7, 3, 7, 7, 6% $(^3P)^4P$
$(^3P)^4D_{1/2}$	69, 53, 48, 54, 50% $(^3P)^4D$ + 11, 30, 0, 5, 12% $(^1D)^2P$ + 12, 5, 31, 28, 26% $(^3F)^4D$ + 3, 7, 0, 2, 5% $(^3P)^2S$ + 2, 4, 0, 0, 0% $(^3P)^4P$ + 2, 1, 17, 8, 4% $(^3P)^2P$ + 1, 0, 4, 3, 3% $(^1S)^2P$

ponent in every ion. Because of this and the inherently impure coupling within the individual ions, for many levels the LS name is useful only as a convenient means of referring to the level.

In Table 4 we compare the observed values of the spin–orbit parameter ζ_{3d} for the $3d^9$ configuration with those calculated with the HF program of Froese-Fischer.[19] In Table 5 we give a similar comparison for the $3p^53d^{10}$ configuration.

In Table 6 the values of the energy parameters obtained at NBS from least-squares fits to the observed $3d^84p$ levels are compared with the HF values. The least-squares calculations include the parameters $\alpha_1(3d3d)$ and $\alpha(3d4p)$ for effective electrostatic interactions within the $3d^8$ core and between the $3d^8$ core and the $4p$ electron. The former has matrix elements $\alpha_1 L_1(L_1+1)$, where L_1 is the total orbital angular momentum of the $3d^8$ core; the latter has matrix elements $\alpha L(L+1)$, where L is the total orbital angular momentum.

The percentage compositions for Sr XII, Zr XIV, and Mo XVI calculated with the fitted values of the parameters are given in Table 7. As was already mentioned, the average purities in the LS scheme are low. The purities in both the J_1j and the J_1l schemes are similarly low. The values of unobserved $3d^84p$ levels calculated with the fitted parameter values are given in parentheses in Table 3. Inasmuch as none of the levels with $J = 9/2$ or $J = 11/2$ has an allowed transition to the $3d^9$ ground configuration, the values for these levels are all necessarily calculated. Most of the other unobserved levels are $J = 1/2$ levels whose transitions to $3d^9\ ^2D_{3/2}$ are calculated to be very weak. For Sr XII no $J = 1/2$ levels were observed.

DISCUSSION

Our $3d^9$–$3d^84p$ line identifications for Sr XII–Nb XV are entirely new. Our wavelengths for Mo XVI are higher than those of Burkhalter *et al.*[7] by about 0.007 Å on the average. Considering that the wavelength uncertainty of Burkhalter *et al.*[7] was ±0.010 Å and that our present uncertainty is ±0.005 Å, the wavelengths are in satisfactory agreement. Five of the Mo XVI lines in Table 1 were not observed by Burkhalter *et al.*[7] Three of the lines listed by them were not observed by us. The identifications of seven lines have been changed.

As is seen in Table 6, the effective parameters $\alpha_1(3d3d)$ and $\alpha(3d4p)$ are small and poorly defined. The effective parameter for the core $\alpha_1(3d3d)$ decreases though the sequence. This is the same trend as that found for the $3d^8$ configuration of the Fe I sequence.[9] In the Co sequence $\alpha_1(3d3d)$ has its maximum value[17,18] at about Kr X. This may be the consequence of a perturbation of the $3p^63d^84p$ configuration by $3p^53d^{10}$, which is nearly coincident in energy in this ion. In Sr XII the $3p^63d^8(^1D)4p\ ^2P_{3/2}$ level appears to be perturbed by $3p^53d^{10}\ ^2P_{3/2}$, and we therefore omitted it from the least-squares fit.

A point of some interest is the crossing of the $(^3F)^2F_{5/2}$ and $(^3P)^4P_{5/2}$ levels between Zr XIV and Nb XV. Although these levels have the same J value, there is no evidence of a perturbation caused by their closeness in energy. A more complicated crossing occurs for the $(^3P)^4D_{1/2}$ and $(^1D)^2P_{1/2}$ levels. The $(^3P)^4D_{1/2}$ level is calculated to lie above $(^1D)^2P_{1/2}$ in Sr XII and Y XIII but below it in Zr XIV, Nb XV, and Mo XVI. However, the eigenvectors of these two levels do not change smoothly through the sequence. The percentage compositions for these two levels in all five ions are given in Table 8, where abrupt changes in composition are evident. In Y XIII–Mo XVI a transition to $3d^9$ is observed from the lower of these two levels but not from the upper. Thus, in spite of the crossing, it is always the lower of the two levels that is observed.

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Revised $3p^63d^8\ ^1S_0$ level of Sr XIII, Y XIV, Zr XV, Nb XVI, and Mo XVII

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Following an observation by Wyart *et al.* [Phys. Scr. **26**, 141 (1982)], we have revised the position of the $3p^63d^8\ ^1S_0$ level in Sr XIII, Y XIV, Zr XV, Nb XVI, and Mo XVII and have redetermined the $3p^63d^8$ energy parameters in these ions.

Recently, Reader and Ryabtsev[1] analyzed the $3p^63d^8$–$3p^53d^9$ transitions in the isoelectronic ions Sr XIII–Mo XVII. In this analysis the $3p^63d^8\ ^1S_0$ level was established by the single transition $3p^63d^8\ ^1S_0$–$3p^53d^9\ ^1P_1$. Subsequently, $3p^63d^9$–$3p^63d^84p$ transitions were analyzed in Sr XII–Mo XVI by Ryabtsev and Reader[2] and in Y XIII–Ag XXI by Wyart *et al.*[3] In their report Wyart *et al.*[3] noted that the parameters for the $3p^63d^8$ core of the $3p^63d^84p$ configuration differed in some important respects from those of the $3p^63d^8$ configuration of the next ion. They concluded that the differences were due to an incorrect $3p^63d^8\ ^1S_0$ level for the ions Sr XIII–Nb XVI in Ref. 1. Further, they proposed new identifications for the $3p^63d^8\ ^1S_0$–$3p^53d^9\ ^1P_1$ transitions in Y XIII–Nb XVI.

We have reviewed our spectra in this regard and have found transitions of the type $3p^63d^8\ ^1S_0$–$3p^53d^9\ ^3D_1$ that support the proposed identifications of Wyart *et al.*[3] A $3p^63d^8\ ^1S_0$–$3p^53d^9\ ^3D_1$ transition was present in our original array for Mo XVII, but it was not included in Ref. 1 because of its apparent absence in the isoelectronic spectra. On the basis of revised calculations for the $3p^63d^8$ configuration we have also revised the $3p^63d^8\ ^1S_0$–$3p^53d^9\ ^1P_1$ identification in Sr XIII. The lines identified as $3p^63d^8\ ^1S_0$–$3p^53d^9\ ^1P_1$ Y XIV–Nb XVI in Ref. 1 are actually $3p^63d^7$–$3p^53d^8$ transitions of the next higher stage of ionization, that is, of manganeselike ions.[4]

In Table 1 we give the $3p^63d^8\ ^1S_0$–$3p^53d^9\ ^1P_1$ and $3p^63d^8\ ^1S_0$–$3p^53d^9\ ^3D_1$ transitions in the ions Sr XIII–Mo XVII. The revised positions of the $3p^63d^8\ ^1S_0$ level in these ions are given in Table 2. The revision of $3p^63d^8\ ^1S_0$ in Mo XVII is due to our inclusion of the $3p^63d^8\ ^1S_0$–$3p^53d^9\ ^3D_1$ transition in the array, which produces a slightly different average value for the $3p^63d^8\ ^1S_0$ level.

The revised energy parameters for the $3p^63d^8$ configuration are given in Table 3. The ratios of the fitted value of $F^4(3d3d)$ to the Hartree–Fock (HF) value, which previously[1] varied from 0.844 for Sr XIII to 0.907 for Mo XVII, are now nearly constant through the sequence. The values of $\alpha(3d3d)$, which previously[1] varied from 203 cm^{-1} for Sr XIII to 123 cm^{-1} for Mo XVII, are also now nearly constant through the sequence. The differences between the observed level values and those calculated with the revised energy parameters are given in Table 4. The percentage compositions obtained with the revised parmeters do not differ significantly from those of Ref. 1 and are therefore not given here.

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Table 1. $3p^63d^8\ ^1S_0$–$3p^53d^9\ ^1P_1$ and $3p^63d^8\ ^1S_0$–$3p^53d^9\ ^3D_1$ Transitions in the Ions Sr XIII–Mo XVII[a]

	Sr XIII		Y XIV		Zr XV		Nb XVI		Mo XVII	
Transition	λ(Å)	Int.	λ(Å)	Int.	λ(Å)	Int.	λ(Å)	Int.	λ(Å)	Int.
$3p^63d^8\ ^1S_0$–$3p^53d^9\ ^1P_1$	88.915	30	84.180	40	79.830	20	75.828	15	72.092	20
$3p^63d^8\ ^1S_0$–$3p^53d^9\ ^3D_1$	–	–	94.186	10	89.853	15	85.938[b]	60	82.317	10

[a] Intensities are visual estimates of photographic blackening.
[b] Blended with $4p\ ^2P_{3/2}$–$6s\ ^2S_{1/2}$ transition of Nb XIII.

Table 2. $3p^63d^8\ ^1S_0$ Levels of Sr XIII–Mo XVII (in cm^{-1})

Configuration	Term	J	Sr XIII	Y XIV	Zr XV	Nb XVI	Mo XVII
$3p^63d^8$	^1S	0	136 720	146 020	155 800	166 070	176 680

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Table 3. Energy Parameters (in cm^{-1}) and Mean Errors Δ of Least-Squares Fits for the $3p^63d^8$ Configurations of Sr XIII, Y XIV, Zr XV, Nb XVI, and Mo XVII[a]

Ion	Parameter	HF	Fitted	Fitted/HF
Sr XIII	E_{av}	36 440	34 047 ± 110	
	$F^2(3d3d)$	214 978	195 749 ± 886	0.911 ± 0.004
	$F^4(3d3d)$	136 981	123 012 ± 814	0.898 ± 0.006
	$\alpha(3d3d)$		121 ± 20	
	ζ_{3d}	6 133	6 103 ± 124	0.995 ± 0.020
	Δ		292	
Y XIV	E_{av}	39 578	37 084 ± 114	
	$F^2(3d3d)$	225 641	206 447 ± 928	0.915 ± 0.004
	$F^4(3d3d)$	143 929	129 622 ± 856	0.901 ± 0.006
	$\alpha(3d3d)$		124 ± 21	
	ζ_{3d}	7 196	7 127 ± 129	0.990 ± 0.018
	Δ		304	
Zr XV	E_{av}	42 883	40 376 ± 121	
	$F^2(3d3d)$	236 241	216 969 ± 987	0.918 ± 0.004
	$F^4(3d3d)$	150 838	136 286 ± 913	0.904 ± 0.006
	$\alpha(3d3d)$		120 ± 22	
	ζ_{3d}	8 388	8 284 ± 134	0.988 ± 0.016
	Δ		320	
Nb XVI	E_{av}	46 430	43 937 ± 125	
	$F^2(3d3d)$	246 787	227 526 ± 1027	0.922 ± 0.004
	$F^4(3d3d)$	157 711	142 891 ± 957	0.906 ± 0.006
	$\alpha(3d3d)$		118 ± 23	
	ζ_{3d}	9 717	9 596 ± 132	0.988 ± 0.014
	Δ		330	
Mo XVII	E_{av}	50 238	47 730 ± 118	
	$F^2(3d3d)$	257 286	238 000 ± 971	0.925 ± 0.004
	$F^4(3d3d)$	164 554	149 128 ± 914	0.906 ± 0.006
	$\alpha(3d3d)$		123 ± 22	
	ζ_{3d}	11 195	11 081 ± 116	0.990 ± 0.010
	Δ		311	

[a] The value for E_{av} listed in the HF column is that obtained by diagonalizing the energy matrix with the HF parameters, $^3F_4$ level set at zero.

Table 4. Differences Observed Minus Calculated (in cm^{-1}) between Observed Level Values and Those Calculated with the Fitted Values of the Parameters for the $3p^63d^8$ Configurations of Sr XIII, Y XIV, Zr XV, Nb XVI, and Mo XVII

Configuration	J	Term	Sr XIII	Y XIV	Zr XV	Nb XVI	Mo XVII
$3p^63d^8$	0	^3P	170	110	80	0	20
		^1S	80	80	70	70	70
	1	^3P	130	200	210	260	220
	2	^3F	210	160	120	90	0
		^3P	−270	−310	−310	−270	−230
		^1D	−360	−330	−330	−330	−290
	3	^3F	170	250	340	380	420
	4	^3F	−100	−110	−150	−180	−140
		^1G	−60	−50	−40	−50	−30

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M E M O R A N D U M
On Cooperation Between the US National Bureau of Standards
and
the USSR Academy of Sciences

In accordance with the US-USSR Agreement on Cooperation in the Fields of Science and Technology, dated July 8, 1977, the US National Bureau of Standards and the USSR Academy of Sciences, referred to below as the Sides, desiring to facilitate the expansion of scientific cooperation for mutual benefit to the two Sides, have agreed as follows:

Article 1

Scientific cooperation may be conducted in the fields of thermal physics and thermodynamics, materials science, spectroscopy, chemistry and chemical kinetics, and cryogenic science. Other fields may be additionally included by mutual agreement.

This cooperation will be carried out pursuant to, and within the framework of, the US-USSR Agreement on Cooperation in the Fields of Science and Technology.

Article 2

Such cooperation may be implemented by exchange of scientists, exchange of scientific and technical information and documentation, joint meetings and seminars, joint research projects, and by other means as may be mutually agreed.

Article 3

Each Side shall designate a coordinator for determining the scientific directions of the cooperation and for ensuring the scientific usefulness of this cooperation.

Article 4

The Sides agree to exchange up to five scientists annually from each Side, with a total length of stay of up to 14 man-months, for carrying out joint research, and also to exchange up to 10 leading specialists from each Side representing the scientific disciplines listed in Article 1 of this Memorandum, for a total length of stay of up to 6 man-months.

Article 5

The selection of scientists described in Article 4 rests with the sending Side, and all visits will be undertaken subject to acceptance by the receiving Side. In addition, each Side may suggest scientists it would like to receive from the other Side within Article 4, and each Side, insofar as possible, will take into account these desires of the other Side.

Article 6

Exchange of scientists and other activities under this Memorandum will be conducted on a receiving-side-pays basis, which means:

1. The receiving Side will assume the expenses for receiving scientists and will pay:

a) per diem in the amount of 12 rubles in the USSR and, correspondingly, the equivalent in dollars in the US for each day of the visit;

b) lodging in a hotel or the provision of an apartment;

c) travel expenses within the country in accordance with the program of visits;

d) emergency medical care, including emergency dental care;

e) expenses for automobile transportation for meeting and seeing off;

2. Expenses for transportation to and from the main destination, which as a rule will be Washington or Moscow, will be borne by the sending Side.

3. Each Side will provide scientists of the other Side the opportunity to conduct scientific research work in laboratories and libraries without cost.

4. Expenses for procuring materials, apparatus, literature, photocopies, and microfilm, which are essential for the completion of the agreed plan of work by scientists of the other Side will be borne by the receiving Side.

5. The receiving Side will not pay expenses for the stay of members of the family of visiting scientists in the receiving country.

Article 7

Nominations of scientists for exchange visits will be submitted to the receiving Side no later than four months before the proposed date for starting the visit. For each scientist nominated, the sending Side will provide the following information: the full name of the scientist, date and place of birth, education and academic degrees, place of work, scientific speciality, a list of the main scientific works and publications, the proposed program of scientific work with a suggested list of the scientific establishments or laboratories to be visited and the scientists to be met, knowledge of foreign languages, topics of lectures that could be delivered by the scientist, proposed date of arrival, and the length of stay.

Article 8

The Receiving Side will respond to this nomination no later than three months after its receipt. If the nomination is acceptable, the receiving Side will inform the sending Side of a possible date of arrival of the scientist in the country and will give its agreement to the program or will propose alternatives to the program.

After receiving the consent of the receiving Side to accept a given scientist, the sending Side shall inform the receiving Side by telegram or telex, two weeks or more in advance, of the exact date of the arrival of the scientist in the country.

Article 9

The receiving Side will facilitate the timely receipt of visas by the scientists of the other Side traveling in accordance with this Memorandum.

Article 10

The National Bureau of Standards authorizes its Office of International Relations, and the USSR Academy of Sciences authorizes its Foreign Relations Department, to conduct administrative affairs in connection with this cooperation.

Article 11

This Memorandum shall enter into force upon signature by both Sides and shall remain in force for five years. Additions and modifications may be made to it, and its period of validity extended, by mutual agreement of the Sides, and with the concurrence of the Executive Agents designated in Article VII of the US-USSR Agreement on Cooperation in the Fields of Science and Technology.

DONE at Moscow this 13th day of December, 1978, in duplicate, in the English and Russian languages, both equally authentic.

For the US National Bureau of Standards

E. Ambler

Director

For the USSR Academy of Sciences

Велихов

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