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# **WITHDRAWAL SHEET**

# **Ronald Reagan Library**



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NATIONAL SECURITY COUNCIL WASHINGTON, O.C. 20506

January 26, 1984

**,CONFIBfilN'ffAis** 

MEMORANDUM FOR MR. CHARLES HILL Executive Secretary Department of State

**SUBJECT:** Renewal of the Memorandum of Cooperation between the US National.Bureau of Standards and the Academy of Sciences of the USSR (C)

The recommendation that we propose to the Soviets the extension of the Memorandum of Cooperation between the U.S. National Bureau of Standards and the USSR Academy of Sciences for five years has<br>been approved. (C) been approved.

• *<u>Potent M.</u> ((month)*<br>Robert M. Kimmitt

Robert M. Kimmitt Executive Secretary

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MEMORANDUM

# NATIONAL SECURITY COUNCIL

# **eeHFIBEHlfIAfi**

January 23, 1984

ACTION

MEMORANDUM FOR **ROBERT C. MCFARLANE JACK MATLOCKAW** 

FROM:

SUBJECT: Renewal of Memorandum of Cooperation Between NBS and USSR Academy of Sciences

The 1978 Memorandum of Cooperation between the National Bureau of Standards (NBS) and the USSR Academy of Sciences was to have expired on December 12, 1983, unless it was modified or extended by mutual agreement. Although a cleared interagency position was not forwarded to us before the expiration date, informal soundings with the Soviets have indicated that they will agree to extend the memorandum, despite its formal expiration, if we wish to do so. NBS recommends that it be extended for a five-year period and State concurs (Tab I). The intelligence community and OSTP believe that the agreement poses no risk of technology loss under the conditions by which it is currently managed. Each project is subject to interagency review from the standpoint of technology transfer before it is approved.

Since renewal of the agreement is consistent with NSDD-75 and supports our policy of maintaining a broad dialogue with the Soviets,  $\chi$  recommend that a five-year extension be approved.

Don Fortier and John Lenczowski concur.

# **RECOMMENDATION:**

That you approve the Kimmitt to Hill Memorandum at Tab II which authorizes renewal of the NBS-USSR Academy Memorandum of Cooperation for five years.

Approve SCM

Disapprove

Attachments:

Tab I Tab II Memorandum from State Memorandum to State

• **€0Nf'IBEHlfIAl:.** , Declassify on: OADR

**DECLASSIFIED NLRR<sub>F06-114/11<sup>#</sup>12280**</sub>

**BY** KML **NARA DATE 6/2/11** 

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United States Department of State

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*Washington, D.C. 20520* 

January 5, 1984

CONFIDENTIAL

MEMORANDUM FOR MR. ROBERT C. MCFARLANE THE WHITE HOUSE

SUBJECT: Renewal of the Memorandum of Cooperation between the US National Bureau of Standards and the Academy of Sciences of the USSR

The 1978 Memorandum of Cooperation between the National Bureau of Standards and the Soviet Academy of Sciences effectively will have expired on December 12, 1983, unless it is modified dr extended by mutual agreement of the two Sides (the Bureau and the Academy) with the concurrence of the Executive Agencies (the Office of Science and Technology Policy and the USSR State Committee for Science and Technology, as designated under the US-USSR Agreement on Cooperation in the Fields of Science and Technology) .

# **BACKGROUND**

Official science and technology exchanges with the Soviet Union have been cut back substantially on two occasions -- in 1980 in response to the Soviet invasion of Afghanistan and in December 1981 when, as part of the sanctions taken against the USSR for its actions in Poland, the President announced that three agreements (space, energy, and science and technology) would be allowed to lapse in 1982. Even though the NBS-Soviet Academy Memorandum referred to the Science and Technology (S&T) Agreement, the Department of State determined that, per the provisions of Article VIII of the S&T Agreement, the validity of the NBS-ASUSSR Memorandum was not effected by the termination of the S&T Agreement. Therefore, requests to continue activities were reviewed on a case-by-case basis through: the interagency mechanism that the U.S. Government had established. A number of activities have been approved on the basis that NBS acquisition of information under the program was considered beneficial to American interests. Since the expiration of the S&T Agreement in July 1982, consistent with our policy (made explicit in NSDD-75) not to dismantle further the framework of exchanges, the U.S. Government decided to renew bilateral agreements in agriculture (1982) and atomic energy (1983) and was negotiating the renewal of the Transportation Agreement when the KAL incident brought these discussions to an end.

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It is the assessment of the National Bureau of Standards (NBS) that the Memorandum with the Soviet Academy has resulted in tangible benefits to the United States and should be extended. Based on the present system of review of all Soviet applicants for cooperative research at NBS, the intelligence community and the Office of Science and Technology Policy believe that this bilateral agreement does not pose a risk of technology loss under the conditions by which it is currently managed.

# **STATE'S VIEWS**

The Department concurs in the assessment by the National Bureau of Standards that the Memorandum should be extended for another five-year period without modification of the operative language of the agreement. Compared with the level of activities under the bilateral agreements in atomic energy, environment, and health and artificial heart research, the NBS program is fairly small in scope and funding.

Given the controls which are currently exercised over the US-Soviet S&T exchanges, we consider that technology transfer concerns have been and will continue to be adequately addressed through existing procedures. All activities are subject to a case-by-case review to minimize possible technology loss.

State notes that in proposing the extension of the Memorandum, the USG is softening, in a sense, the practical consequences of allowing the expiration in 1982 of the S&T Agreement and that this could be incorrectly interpreted by the Soviets to mean that we do not have a firm policy in regard to scientific exchanges. However, in the case of· the NBS Memorandum, State is of the opinion that the scientific and intelligence benefits to the United States of continuing the activities under the Memorandum outweigh any possible Soviet misreadings of our intentions. The renewal of the Memorandum is in line with the policy formally enunciated in NSDD-75 in January 1983. On political grounds, consistent with this policy that the "U.S. should not further dismantle the framework of exchanges," it would be in the U.S. interest to extend the NBS-Soviet Academy Memorandum.

In terms of our overall relationship with the Soviet Union, an extension of the Memorandum would provide us some flexibility to adjust the tightening or relaxing of our

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exchanges policy to future shifts in the political situation. We follow this approach under other agreements where we are continuing with certain routine exchanges, particularly in areas relating to health, pollution control, and housing construction.

For their part, the Soviets have indicated at senior levels a clear interest in extending the Memorandum. Early this year, Academy Vice President Velikhov suggested that the Academy would be interested in an extension if NBS were.

As in our other S&T exchange programs, the activities conducted pursuant to the Memorandum afford our visiting American specialists with opportunities not otherwise available to gain access to Soviet scientists and facilties and to keep abreast of Soviet developments and efforts in basic research. This is of clear benefit scientifically to the United States. The framework of the Memorandum also provides opportunities for our visiting researchers to engage in informal dialogue with their Soviet colleagues on U.S. positions on a wide range of topics, paramount among them the American displeasure at the continuing repression of many Soviet scientists.

# **STATE'S RECOMMENDATION**

State recommends that we propose to the Soviets that the Memorandum be extended for a five-year period.

Charles Hi Executive Secretary

Attachments:

- 1. EUR/IG Report on the Extension of the Memorandum of Cooperation between the US National Bureau of Standards and the USSR Academy of Sciences
- 2. NBS Evaluation
- 3. Memorandum of Cooperation between the US National Bureau of Standards and the USSR Academy of Sciences

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# **NLRR**  $F06 - 114/11 \stackrel{1}{\sim} 12283$

# **BY KML NARA DATE**  $5/2/11$

EUR/IG REPORT ON THE EXTENSION OF THE MEMORANDUM OF COOPERATION BETWEEN THE US NATIONAL BUREAU OF STANDARDS AND THE USSR ACADEMY OF SCIENCES

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The 1978 Memorandum of Cooperation between the National Bureau of Standards (NBS) and the Soviet Academy of Sciences will expire automatically on December 12, 1983. A new agreement extending or amending the current agreement will be required if we are to continue cooperation in this area.

The Memorandum was signed at Moscow by NBS Director Ernest Ambler and Academy Vice President Ye. P. Velikhov on December 13, 1978, with a period of validity of five years. The Memorandum has the status of an implementing arrangement under the US-USSR Agreement on Cooperation in the Fields of Science and Technology (S&T), signed on May 24, 1972. The umbrella S&T Agreement, along with cooperative agreements in space and energy, were allowed to lapse in 1982 in accordance with the President's December 1981 announcement of sanctions against the Soviet Union in response to the imposition of martial law in Poland. Despite the non-renewal of the S&T Agreement, it was determined by the Department of State that activities under the NBS-ASUSSR Memorandum should continue because NBS acquisition of information under the program was considered beneficial to American interests and that, as an implementing arrangement, the Memorandum would not be legally affected by the expiration of the umbrella agreement.

The Memorandum, which provides- for collaboration in the basic sciences between NBS and various research institutes of the Soviet Academy, specifically mentions cooperation in the fields of thermal physics and thermodynamics, materials science, spectroscopy, chemistry and chemical kinetics, and cryogenic science. There are presently five applications pending for exchange visits under this program. The Soviet proposals are in the fields of atomic and molecular spectroscopy, while the NBS proposals are in chemical thermodynamics and measurement methodology for non-ionizing electromagnetic readiation. NBS anticipates significant scientific benefit from the American proposals, with particular interest in the last-mentioned because of the wide difference between current US and USSR exposure standards in this area.

# **SUMMARY CONCLUSIONS AND AGENCY RECOMMENDATIONS**

The National Bureau of Standards' evaluation indicates:

--The cooperative program with the Soviet Academy has provided direct, significant scientific benefit to ongoing projects at NBS through not only the usual collaboration with

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Soviet scientists, but as well through first-hand study of the details of Soviet experimental techniques not ordinarily accessible without this bilateral program.

--With the expiration of the umbrella S&T agreement, the NBS memorandum provides access to Soviet research facilities not possible under the remaining official bilateral science agreements.

--The program has progressed on a modest and selective scale at an annual cost to NBS of from \$8 to 12 thousand annually and has yet to reach the upper exchange limits noted in the Memorandum.

--NBS scientists have generally been provided the access to laboratory facilities as requested in their exchange proposals. However, in a recent case when the Soviets failed to provide already agreed-upon arrangements and laboratory visits, NBS notified the Academy that the applications of three Soviet scientists to visit NBS under the Memorandum would not be processed until an explanation was provided.

--In its appraisal of applications for exchange visits, NBS pays particular attention to the questions of reciprocity, mutual benefit, scientific soundness, and any potential for significant technological loss. Subject areas are limited to those considered to be basic rather than applied research. Soviet applications are screened by the Committee on Exchanges (COMEX) to obtain a thorough appraisal of any potential for undesired technology loss.

NBS, as set forth in its report (attached), recommends that the Memoradum be renewed without modification of the text for a period of five years.

State recommends proposing an exchange of notes with the Soviets providing for a five-year extension. State agrees with NBS that there is no need to modify the existing language of the Memorandum.

Consistent with the policy directive NSDD-75, State believes that while we should continue to monitor the overall level of S&T exchanges in response to soviet actions, we should not futher dismantle the framework which now exists. As in our

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other S&T exchange programs, the activities conducted pursuant to the NBS-ASUSSR Memorandum scientifically benefit NBS programs, afford our visiting scientists access to laboratory facilities not otherwise available to study specialized Soviet research techniques, and keep Americans abreast of developments in Soviet science.

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State notes, however, that in proposing the extension of the Memorandum, the U.S. Government is softening, in a sense, the practical consequences of allowing the expiration in 1982 of the Agreement on Cooperation in the Fields of Science and Technology: This could be incorrectly interpreted by the Soviets to mean that we do not have a firm policy in regard to scientific exchanges. However, in the case of the NBS Memorandum, State is of the opinion that the scientific and intelligence benefits to the United States of continuing the activities under the Memorandum outweigh any possible Soviet misreadings of our intentions. The renewal of the Memorandum is consistent with the policy of the USG as set forth in NSDD-75.

The Committee on Exchanges (COMEX) recommends that the National Bureau of Standards be permitted to extend its Memorandum and believes that NBS has done a good job of guarding against significant technology loss. COMEX will continue to review the program proposals on a case-by-case basis.

The Office of Science and Technology Policy (OSTP) concurs in the NBS proposal to extend the Memorandum for five years provided that the exchange proposals continue to be reviewed for possible technology transfer concerns as is presently being done.

The Arms Control and Disarmament Agency, National Aeronautics and Space Administration, National Science Foundation, and Department of the Interior concur in the renewal of the Memorandum for five years.

Other agencies offered no comment.

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 $|228|$   $2$ **UNITED STATES DEPARTMENT OF COMMERCE** /O **National Bureau of Standard•**  Washington, D.C. 20234

**NOV 16 1983** 

MEMORANDUM FOR Byron Morton Deputy Director, EUR/SOV Department of State Department of State<br> **Prom:** Edward L. Brady Edward F. Brady<br> **Associate Director for** 

**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 teminate 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 infomation 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

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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 nonrenewal 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 aide 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 agreedupon 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.

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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.

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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<sup>6</sup> 3d<sup>8</sup>-3p<sup>5</sup> 3d<sup>9</sup> 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 3p5 3d9 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 A. 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.* <sup>1</sup>

**The** 3p6 3d8-3p5 3d9 transitions in Y XIV, Zr xv, Nb·XVI, and Mo XVII were investigated recently by Bogdanovichene *et al.*<sup>2</sup> 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.*<sup>3</sup> 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 lowinductance 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<sup>6</sup> 3d<sup>8</sup> and  $3p<sup>5</sup>3d<sup>9</sup>$  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 A. As several important transitions for the present ions were expected to lie below 70 A, 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 A. 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 I. The uncertainty of the wavelengths is  $\pm 0.005$  Å. For perturbed lines the uncertainty is  $\pm 0.010$  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 TIIE **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.<sup>2</sup> The  $3p^6$  3d<sup>8</sup> levels included  ${}^3F_{2,3,4}$ ,  ${}^3P_{1,2}$ , and  ${}^1D_2$ . The  $3p^5$  3d<sup>9</sup> levels included  ${}^{3}F_{2,3,4}$ ,  ${}^{3}P_{1,2}$ ,  ${}^{3}D_{1,2,3}$ , and  ${}^{1}D_2$ . These levels were confirmed by additional combinations found in the present observations. The levels  $3p^6$   $3d^8$ <sup>3</sup> $P_0$ ,  $^1G_4$ ,  $^1S_0$ , and  $3p^{5}$  3d<sup>9</sup>  $3P_0$ ,  $1F_3$ , and  $1P_1$ , which previously<sup>2</sup> 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.<sup>9</sup> 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.

# **3pl 3cl'** 1P1

This level had been established by a single transition in each ion,  ${}^{1}D_{2}$ <sup>1</sup> $P_1$ . Our new low-wavelength data provided the <sup>3</sup> $P_2$ <sup>-1</sup> $P_1$  combinations, confirming the previous identifications in Y, Zr, and Mo. For Nb XVI the previous  ${}^{1}D_{2}{}^{-1}P_{1}$  identification (70.474 **A) was** replaced by a line at 70.718 A, resulting in a revised value for  $3p^5 3d^9 1p_1$ .

# $3p^2 3d^2 1$ **G** and  $3p^5 3d^2 1$ **F**<sub>2</sub> **3d**<sup>2</sup> **1F**<sub>2</sub>

identification was listed<sup>2</sup> as doubtful in Y and Zr and was the highest predicted line strength within the present array.<br>
absent in Nb and Mo. We have now replaced these identifi- In Ref. 2 these levels were connected to absent in Nb and Mo. We have now replaced these identifi-<br>
cations with those given in Table 1, which includes values for through the single transition  ${}^{1}G_{4}{}^{-3}D_{3}$ . We have now replaced cations with those given in Table 1, which includes values for through the single transition  ${}^{1}G_{4}{}^{-3}D_{3}$ . We have now replaced<br>Nb and Mo as well. These lines were the most prominent the  ${}^{1}G_{4}{}^{-3}D_{3}$  identific Nb and Mo as well. These lines were the most prominent the  ${}^1G_4-{}^3D_3$  identifications with those given in Table 1. This unidentified lines in the expected region and, although there in turn revises the  ${}^1G_4$  and unidentified lines in the expected region and, although there in turn revises the  ${}^{1}G_4$  and  ${}^{1}F_3$  level values. The new values are no confirming transitions, there is little doubt that the are confirmed by the fou are no confirming transitions, there is little doubt that the are confirmed by the four additional combinations,  ${}^{3}F_{3}{}^{-1}F_{3}$ ,<br>identifications are correct. They are strongly supported by  ${}^{3}F_{2}{}^{-1}F_{3}$ ,  ${}^{1}D_{2$ identifications are correct. They are strongly supported by  ${}^{3}F_{2}{}^{-1}F_{3}$ ,  ${}^{1}D_{2}{}^{-1}F_{3}$ , and  ${}^{1}G_{4}{}^{-3}F_{3}$ . The line identified as  ${}^{3}P_{1}{}^{-3}P_{0}$ , the least-squares calculations.

The  ${}^{1}G_{4}$ - ${}^{1}F_{3}$  transition is easily identified as an intense line This level was based on the single transition  ${}^{1}S_{0}{}^{-1}P_{1}$ . The on the low-wavelength side of the transition group.<sup>2,3</sup> It has identification was listed<sup>2</sup> as doubtful in Y and Zr and was the highest predicted line  ${}^{1}G_{4}$ - ${}^{3}D_{3}$  in Y XIV was previously identified as  ${}^{3}P_{1}$ - ${}^{3}P_{0}$ .



 $\overline{\phantom{a}}$ .



• Symbols: bl, blend of **two linea;** h, hazy; p, perturbed by cloee line.

<sup>b</sup> Present value for line given originally by Bogdanovichene et al., Ref. 2.

• Present value for line given originally by Bogdanovichene *et al.*, Ref. 2, and by Burkhalter *et al.*, Ref. 3.

" Present value for line given originally by Bogdanovichene et al., Ref. 2, revised classification.

• Doubly clauified. *I* Blended with 96. 731 *J,,,* of Ti. (The Sr espoaures were made with an anode of Sr and • cathode of Ti.)

• Blended with **a** line of Zr XII; - Ref. 7.

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Table 2. Energy Levels (in cm<sup>-1</sup>) of the  $3p^4 3d^3$  and  $3p^5 3d^3$  Configurations of Sr XIII, Y XIV, Zr XV, Nb XVI, and Moxvn

• New level; all levels for Sr XIII are new.

# **3p5 3d' ~Po**

This level makes only one combination within the present array,  ${}^{3}P_{1}$ - ${}^{3}P_{0}$ . 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 par**ticularly strong because there is no other possible choice within a reasonable distance of the predicted position and, furthermore, the other member of the blend,  ${}^{3}F_{3}$ <sup>-3</sup> $F_{3}$ , appears to be anomalously strong compared with its **appearance**  elsewhere in the sequence.

# $3p^5 3d^3 P_0$

This level can make three transitions, of which two,  ${}^{3}P_{0}$  ${}^{3}P_{1}$ and  ${}^{3}P_{0}$ - ${}^{3}D_{1}$ , are expected to be reasonably strong and one,  ${}^{3}P_{0}$ - ${}^{1}P_{1}$ , is expected to be weak. In Ref. 2, values for  ${}^{3}P_{0}$  were



Fig. 1. Structure of the 3p<sup>6</sup> 3d<sup>8</sup> configuration of Mo XVII.



Fig. 2. Structure of the  $3p^5$  3d<sup>9</sup> configuration of Mo XVII. Levels are grouped into *LS* terms.



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

given for Y, Zr, and Nb based on the single transition  ${}^{3}P_{0}$ - ${}^{3}D_{1}$ . No value was given for Mo. We have now observed the  ${}^{3}P_{0}$ - ${}^{3}D_{1}$  as well as the  ${}^{3}P_{0}$ - ${}^{3}P_{1}$  transition for the present ions, confirming the previous identifications and providing values for Mo. In Y the  $3p^6$  3d<sup>8</sup>  $3P_0$  and  $3P_1$  levels are nearly coincident and the  ${}^{3}P_{0}$ - ${}^{3}P_{1}$  and  ${}^{3}P_{1}$ - ${}^{3}P_{1}$  transitions thus cannot be resolved. Our value for  ${}^{3}P_{0}$ - ${}^{3}D_{1}$  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  ${}^{3}P_{1}$ - ${}^{3}P_{0}$  as a fairly strong line in Sr further supports the proposed blend of  ${}^{3}P_{1}$ - ${}^{3}P_{0}$  and  ${}^{3}F_{3}$ - ${}^{3}F_{3}$  in Y.

Finally, we confirm the value for  ${}^{3}F_{3}$ - ${}^{3}D_{2}$  of Mo XVII given in Ref. 2 (75.843 A), compared with the value given in Ref. 3 (75.624 A). 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<sup>10</sup> that minimizes the differences between the observed and calculated **wave** numbers. The uncertainty of the level values is about  $\pm 50$  cm<sup>-1</sup>.





 $\bullet$  The value of  $E_{av}$  listed in the HF column is that obtained by diagonalizing the energy matrix with the HF parameters, <sup>3</sup>F<sub>4</sub> level set at zero.

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The levels of the 3p6 3d8 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 3p6 3d9 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 3p6 3d8 level values by least-squares calculations are





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Table 6. Percentage Compositions Cor the 3p5 3d' Levela of Sr XIII, Zr xv, and Mo XVII

given in Table 3. The HF values of the parameters are also given here. The parameter  $\alpha$  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<sup>-1</sup>. The present values of  $\alpha$  are consistent with the value of 108 cm<sup>-1</sup> obtained by Podobedova *et al.*<sup>11</sup> for the isoelectronic ion Ge VII. A value for  $\alpha$  of 48 cm<sup>-1</sup> was obtained by Meinders<sup>12</sup> 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,  $\alpha$  decreases significantly with increasing ionization.

The ratios of the fitted values of the parameters to the HF

**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							
$3p^6$ $3d^8$	$\bf{0}$	3P	110	100	110	30	10
		1S	$-20$	10	30	40	70
	1	3P	$-110$	10	70	190	220
	$\overline{2}$	3F	220	220	210	180	$-10$
		$_{sp}$	80	$-110$	$-220$	$-250$	$-230$
		1D	$-80$	$-130$	$-180$	$-240$	$-290$
	3	3 <sub>F</sub>	$-90$	30	150	270	420
	4	3F	$-130$	$-110$	$-160$	$-180$	$-150$
		1G	$\bf{0}$	$-10$	$-20$	$-20$	$-40$
$3p^5$ $3d^9$	0	3 <sub>P</sub>	10	100	90	160	120
	$\overline{1}$	зp	$-110$	$-240$	$-280$	$-410$	$-370$
		3D	100	$-10$	$-60$	$-150$	$-220$
		1P	$-30$	$\bf{0}$	30	70	120
	$\overline{\mathbf{2}}$	1D	10	20	30	50	60
		3D	80	150	230	310	340
		$^{3}F$	$-70$	$-110$	$-170$	$-240$	$-290$
		$_{\rm sp}$	90	110	160	200	220
	3	3 <sub>F</sub>	100	120	200	250	330
		$\mathbf{p}$	$-190$	$-140$	$-220$	$-270$	$-360$
		1F	20	10	30	40	70
	4	$^{3}F$	$-30$	$-40$	$-40$	$-20$	0

values shown in Table 3 are generally close to unity. This is surprising because the HF calculation<sup>9</sup> does not include the effects of relativity. The ratios vary smoothly through the sequence.

The percentage compositions for the  $3p^6$  3 $d^8$  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  ${}^{3}P_{2}$  and  ${}^{1}D_{2}$ 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<sup>13</sup> 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<sup>-1</sup>. Addition of  $X^2(3p3d)$  further reduced the mean error to 193 cm<sup>-1</sup>. [When  $X^2(3p3d)$  is added alone, the mean error is reduced only to  $2200 \text{ cm}^{-1}$ . These parameters are thus significant. Their values are nearly constant through the sequence.

The percentage compositions for the 3p<sup>5</sup> 3d<sup>9</sup> configurations of Sr xm, 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  $3p^6$   $3d^8$ <sup>3</sup> $F_2$  and <sup>3</sup> $P_2$ . 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  $3d^{10}4s^2-3d^94s^24p$  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 *3d94s4p* were interpreted simultaneously with a root-mean-square deviation of 122 cm<sup>-1</sup>; forty-four levels of  $3d^94p^2$  were interpreted in the same way with a root-mean-square deviation of  $200 \text{ cm}^{-1}$ . Line identifications and energy levels were obtained for the  $3d^{107}p$  configuration of the Cu-like ions Yx1-Mox1v.

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 mem her of the Cu I isoelectronic sequence, Mo XIV has the ground configuration  $3d^{10}4s$ . Its one-clectron spectrum and those of the neighboring members of the sequence Y XI, Zr XII, and Nb XIII have already been well described.<sup>1-4</sup> In a recent description<sup>5</sup> 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 *3d10-3d94p*  resonance transitions of the Ni-like ion Mo xv were interpreted as *3d104s-3d94s4p* transitions of Mo XIV and 3d<sup>10</sup>4s<sup>2</sup>-3d<sup>9</sup>4s<sup>2</sup>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  $3d^{10}4p-3d^94p^2$  transitions of Mo XIV.

# **EXPERIMENT**

The experimental material for this work was the same as used for a recent study of  $3p^63d^8-3p^53d^9$  transitions of Y XIV, Zr XV, Nb XVI, and Mo XVII.<sup>6</sup> Briefly, the 10.7-m grazingincidence 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 A/mm at the 85° angle of incidence.

# LINE IDENTIFICATIONS AND TIIEORETICAL INTERPRET ATJON

# **3d11.ts-3d'414p Transitions**

As was seen in Mo XIV,<sup>5</sup> the strongest satellite lines are due to  $3d^{10}4s-3d^{9}4s4p$  transitions. We thus interpreted these transitions first. The *3d94s4p* configuration contains 23 levels, of which eleven have  $J = 1/2$  or  $3/2$  and can therefore combine with  $3d^{10}4s$  <sup>2</sup>S<sub>1/2</sub>. Our line identifications were made with the help of theoretical calculations of the 3d<sup>9</sup>4s4p-level structures and *3d104s-3d94s4p* line strengths in the four ions that were investigated. Initial energy parameters for the *3d94s4p* configurations **were** obtained by Hartree-Fock (HF) calculations.<sup>7</sup> After identifying the strongest and mOBt 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 posaible transitions in each ion could be identified. Only the transition  $3d^{10}4s \, {}^{2}S_{1/2}$  -  $3d^{9}(2D)4s4p(1P) \, {}^{2}D_{3/2}$ , 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<sup>5</sup> identification of this transition in Mo XIV is probably spurious.

The wavelengtha and classifications of the identified *3d104s-3d94s4p* transitions are given in Table 1. The uncertainty of the wavelengths is ±0.005 A. 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



Table 1. Lines Classified as  $3d^{10}4s-3d^{9}4s4p$  and  $3d^{10}4p-3d^{9}4p^2$  Transitions in Y XI, Zr XII, Nb XIII, and Mo XIV<sup>c</sup>

		Y xı		ZrX11		Nb xIII		Mo XIV	
Classification	Code	$\lambda(A)$	Int.	$\lambda(A)$	Int	$\lambda(A)$	Int.	$\lambda(A)$	Int
4s ${}^{2}S_{1/2}$ ( ${}^{2}D, {}^{1}P$ ) ${}^{2}P_{1/2}$	A	73.639	15	64.466	20	57.001	15	50.788	10
4p <sup>2</sup> P <sub>3/T</sub> ( <sup>2</sup> D, <sup>1</sup> S) <sup>2</sup> D <sub>5/2</sub>		73.908	$\overline{2}$	64.794	1w	57.393	$\overline{2}$	51.20	1
$4p^{2}P_{1/T}^{*}(^{2}D, {}^{3}P)$ ${}^{4}P_{3/2}$	b	74.175?	1			57.187	1		
4p <sup>2</sup> Pin <sup>(2</sup> D, <sup>3p</sup> ) <sup>2</sup> P <sub>1/2</sub>	c	74.391	5	65,059	$\overline{\mathbf{2}}$	57.468	$\overline{\mathbf{2}}$	51.158	ı
4s ${}^{2}S_{1/2}$ ( ${}^{2}D, {}^{1}P$ ) ${}^{2}P_{3/2}$	B	74.456	30	65.200	50	57.662	30	51.398	20
4p <sup>2</sup> P <sub>1/2</sub> ( <sup>2</sup> D, <sup>1</sup> D) <sup>2</sup> D <sub>2/2</sub>	d	74.896	8	65.466	5	57.797	3	51.434	1
$4p^{2}P_{3/2}^{*}(^{2}D, {}^{1}D)~^{2}F_{5/2}$		74.954	2p	65,540	3	57,884	$\mathbf{2}$	51.531	1
4p <sup>2</sup> P <sub>3/2</sub> ( <sup>2</sup> D, <sup>3</sup> P) <sup>4</sup> P <sub>1/2</sub>	ł			65,609					
4p <sup>2</sup> P <sub>2/T</sub> ( <sup>2</sup> D, <sup>3</sup> P) <sup>4</sup> P <sub>2/2</sub>		75.209	10						
4p <sup>2</sup> Pin <sup>(2</sup> D, <sup>3p</sup> ) <sup>4</sup> F <sub>2/2</sub>	h	75.233	15	65.760	10	58.053	10	51.666	5
4p <sup>2</sup> P <sub>2/2</sub> ( <sup>2</sup> D, <sup>3</sup> P) <sup>2</sup> P <sub>2/2</sub>		75.307	25	65,896	10	58.241	15	51.894	8
4p <sup>2</sup> P <sub>1/2</sub> ( <sup>2</sup> D, <sup>1</sup> D) <sup>2</sup> P <sub>1/2</sub>				65.816?	1				
4p <sup>2</sup> P <sub>2/2</sub> ( <sup>2</sup> D, <sup>3</sup> P) <sup>2</sup> P <sub>1/2</sub>		75.438	10	66.029	5	58.362	5	52.00	2u
4p <sup>2</sup> P <sub>2/2</sub> ( <sup>2</sup> D, <sup>3</sup> P) <sup>2</sup> D <sub>5/2</sub>		75.521	35	66,080	20	58,386	20	52.013	10u
$4p^{2}P_{1/2}^{*}(^{2}D,{}^{3}P)~^{2}D_{3/2}$	m	75.584	25	66.115	10	58.407	10	52.019	<b>8u</b>
4p <sup>2</sup> P <sub>1/2</sub> (2D, <sup>3</sup> P) <sup>4</sup> D <sub>1/2</sub>	n	75.945	$\mathbf{2}$	66.327	$\overline{2}$				
4s ${}^{2}S_{1/2}$ ( ${}^{2}D, {}^{3}P$ ) ${}^{4}D_{3/2}$	C	76.274	25	66,597	8	58.728	10	52.225	5
$4p^{2}P_{1/2}^{*}(^{2}D,{}^{1}D)^{2}P_{3/2}$	$\bullet$	76.283?	2u	66.687?	3	58.888*	5	$52.415*$	$\mathbf{2}$
4p <sup>2</sup> P <sub>3/2</sub> -( <sup>2</sup> D, <sup>3</sup> P) <sup>4</sup> F <sub>5/2</sub>	Þ					58,909	3		
$4p^{2}P_{1/2}^{*}(^{2}D, {}^{1}D)~^{2}S_{1/2}$	a	76.331	10	66.717	5p	58.888*	5	$52.415*$	$\overline{2}$
$4p^{2}P_{3/2}^{*}(^{2}D, {}^{1}D)~^{2}P_{1/2}$	r	76.434?	15l	66,792?	5				
$4p^{2}P_{1/\mathcal{I}}^{*}(^{2}D,{}^{3}P)$ $^{4}D_{3/2}$		76.584?	15						
4s ${}^{2}S_{1/2}$ ( ${}^{2}D, {}^{3}P)$ ${}^{4}D_{1/2}$ )	D	76.66	1	66.928	3	59.016	5w	52.473	5
$4s^{2}S_{1/2}-(^{2}D, ^{3}P)^{2}P_{1/2}^{*}$	Ē	76.843	40	67.121	30	59.214	20	52.687	10
$4s^{2}S_{1/2}$ (2D, 3P) $^{2}P_{3/2}$	F	76.920	50	67.201	50	59.285	40	52.750	20
4s ${}^{2}S_{1/2}$ (2D, 3P) ${}^{2}D_{3/2}$	G	77.340	35	67.569	30	59.612	20	53.044	10
4p <sup>2</sup> P <sub>3/3</sub> ( <sup>2</sup> D, <sup>1</sup> D) <sup>2</sup> P <sub>3/2</sub>	t					59.826	$\mathbf{2}$		
4p <sup>2</sup> P <sub>3/2</sub> ( <sup>2</sup> D, <sup>1</sup> D) <sup>2</sup> S <sub>1/2</sub>	u	77.436	5l						
4s ${}^{2}S_{1/2}$ (2D, 3P) ${}^{4}P_{1/2}$	H	77.667	5.	67.768	5	59.722	5	53.095	3
4s <sup>2</sup> S <sub>1/2</sub> ( <sup>2</sup> D, <sup>3</sup> P) <sup>4</sup> F <sub>3/2</sub>		77,910	5w	68.022	$\mathbf 2$	59.971	5	53.335	3
$4s^{2}S_{1/2}$ ( <sup>2</sup> D, <sup>3</sup> P) <sup>4</sup> P <sub>3/2</sub>	J.	78.424	25	68.476	15	60.383	10	53.725	5

 $\bullet$  Levels are designated in *LS* coupling: The parent terms for 3d<sup>9</sup> 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<sup>104g-3d%4</sup>p-3d%4p transitions; lower-case letters denote 3d<sup>104</sup>p-3d<sup>9</sup>4p<sup>2</sup> transitions. Symbols: u, unresolved; u, wide; i, shaded to longer wavelengths; p, perturbed by close line; °, doubly classified. Lines for which a question mark<br>is given have observed intensities much large- than expected;

the transitions may be written as  $[3d^{10}(^1S)]4s [3d<sup>9</sup>4p(L,S)]$ 4s, the intensities are proportional to the amount of  $[3d^94p^{(1)}]$ 4s  ${}^2P_{1/2}^*$  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  $3d<sup>9</sup>4s4p$  levels involves fitting the ten observed levels with the eight Slater parameters for the  $3d^94s4p$  configuration: A,  $F^2(3d4p)$ ,  $G^1(3d4p)$ ,  $G<sup>3</sup>(3d4p)$ ,  $G<sup>1</sup>(4s4p)$ ,  $G<sup>2</sup>(3d4s)$ ,  $\zeta_{3d}$ , and  $\zeta_{4p}$ . As  $G<sup>3</sup>(3d4p)$ has a constant contribution to the terms having  $J = 1/2, 3/2$ levels  $(2.4P, 2.4D, 4F)$ , 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. Neverthelesa, their variation along the aequence was not completely regular. The irregularities are undoubtedly due to small perturbations that may **be expected** for such high

configurations. For example, the  $3d^{107}p$  configuration overlaps 3d94s4p and, as the relative position of the two configurations varies along the sequence, different repulsion effects may be expected. *AB* 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,  $Z_{\text{av}} = 40.5$ .) However, with this constraint, the coefficient *a* of the linear term in the GLS procedure was undefmed for all parameters except  $G^1(4s4p)$  and  $\zeta_{3d}$ . We thus set  $a$  $= 0$  except for these two parameters, leaving 13 parameters to account for the 40 observed levels. The resultant rootmean-square deviation of this fit, 122 cm-1, is comparable with the uncertainty of the energy-level values, which is about

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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  $Y XIV.<sup>6</sup>$ 

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  $\Delta \sigma = \sigma_{\text{exp}}$  - $\sigma_{\rm calc}$  larger than the experimental uncertainty.

The 3d<sup>9</sup>4s4p energy levels are listed in Table 2. The levels are designated in the  $3d^9(2D)4s4p^{(1,3P^c)}$  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.

## **3d114p-3d'4pZ Transitions**

With the strongest satellite lines accounted for by the 3d<sup>10</sup>4s-3d<sup>9</sup>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<sup>9</sup>4s4p configurations proved to be important.

The  $3d^94p^2$  configuration is expected to lie below the ionization limit in the present ions. It **baa a** total of 28 levela, of which 21 have  $J = 1/2$ ,  $3/2$ ,  $5/2$  and can combine with  $4p$  ${}^{2}P_{1/2.3/2}^{*}$ . Because of strong electrostatic interactions within the  $n = 4$  shell, the  $3d^94p^2$  configuration is expected to be perturbed by the 3d<sup>9</sup>4s<sup>2</sup>, 3d<sup>9</sup>4s4d, and 3d<sup>9</sup>4d<sup>2</sup> configurations, which do not radiate to the 3d<sup>10</sup>nl levels. They show their presence mainly by perturbing the  $3d^94p^2$  levels. The  $3d^94s^2$ and  $3d<sup>9</sup>4d<sup>2</sup>$  configurations are expected to be far enough from  $3d<sup>9</sup>4p<sup>2</sup>$  that their perturbations can be treated by effective electrostatic interactions. However, *3d94s4d* is close to  $3d<sup>9</sup>4p<sup>2</sup>$  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  $3d^94s4d$  and about 10 levels of  $3d^94p^2$  would not be observable with the present data. Ensuing least-squares calculations were made by fixing the internal *3d94s4d* parameters at their HF values. The position of the 3d94s4d configuration relative to *3d94p2* 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  $3d<sup>9</sup>4s4d$  parameters were fixed except the  $3d^94s4d-3d^94p^2$  configuration interaction integral  $R^1(4p4p, 4s4d)$ . Again, a GLS procedure was used for fitting the  $3d^94p^2$  parameters and  $R^1(4p4p, 4s4d)$ . The scaling factors of  $F^2(3d4p)$ ,  $G^1(3d4p)$ ,  $G^3(3d4p)$ ,  $\zeta_{3d}$ , and  $R<sup>1</sup>(4p4p, 4s4d)$  were assumed to be constant along the sequence. Scaling factors for  $F^2(4p4p)$  and  $\zeta_{4p}$  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  $44 \frac{3d^94p^2}{p}$  energy levels in the four ions. The fitted and HF values of the parameters for the  $3d^94p^2$  configurations are given in Tables 4 and 5, respectively. Table 5 also includes the HF values for *3d94s4d.* In the least-squares fits to the observed levels, the  $\alpha L (L + 1)$  correction for the final terms of  $3d<sup>9</sup>4p<sup>2</sup>$  remained undefined and was dropped. The fitted values of *a* for the terms of *4p*2 are given in Table 4. The imal **root-mean-square**  deviation of the calculated values was  $200 \text{ cm}^{-1}$ .

The identified  $3d^{10}4p-3d^94p^2$  transitions are given in Table 1. The  $3d^94p^2$  energy levels are given in Table 6. For designating the levels, no entirely satisfactory coupling scheme could be found. We have adopted the  $(3d^9 S_1 L_1, 4p^2 S_2 L_2)$ SLJ scheme, although it is not appreciably better than the  $(3d^9S_1L_1J_1, 4p^2S_2L_2J_2)$  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





 $\bullet$  The deviations  $\Delta E = E_{\rm{can}} - E_{\rm{th}}$  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  $(2D, 1P)$   $2D_{3/2}$  levels are given in brackets.

\*Level value based on eyepiece measurement; not used in least-squares fit.





 $*$  GLS fit of  $3d^24p^2 + 3d^24d$ .

**• GLS fit of 3d\*4s4p.** 

<sup>1</sup> An equal value has been assumed for the four elements.

<sup>2</sup> The same scaling factor has been assumed for  $G^3(3d4p)$  and  $G^1(3d4p)$ .

<sup>3</sup> 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<sup>107</sup>p<sup>2</sup>P° 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 A) 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  ${}^{2}P_{3/2}^{*}$  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* <sup>2</sup>S<sub>1/2</sub>-7p <sup>2</sup>P<sub>3/2</sub>. If we identify a line at 77.058 Å as  $4s$  <sup>2</sup>S<sub>1/2</sub>-7p  ${}^{2}P_{1/2}^{*}$ , 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  $4s^{2}S_{1/2}-7p^{2}P_{3/2}^{2}$  and 0.0184

if 76.928 **A** is used for this transition. Because of the regularity of *on•* for the lower members of the *np* series (0.0192 for 4p, 0.0188 for 5p, and 0.0187 for Gp), we consider 76.928 Å as the best choice for  $4s \frac{2S_{1/2}-7p}{2P_{3/2}^2}$ . The reduced intensity of  $F$  in  $Y$  XI is undoubtedly caused by mixing between the  $3d^9(2D)4s4p(3P)$   $2P_{3/2}^*$  and  $3d^{107}p$   $2P_{3/2}^*$  states, which makes unambiguous identification of the two lines difficult.

In Mo XIV Curtis *et al.*<sup>8</sup> classified lines at  $53.19 \pm 0.05$  Å and  $53.30 \pm 0.05$  Å as  $4s$  <sup>2</sup>S<sub>1/2</sub>-7p <sup>2</sup>P<sub>3/2</sub> and  $4s$  <sup>2</sup>S<sub>1/2</sub>-7p <sup>2</sup>P<sub>1/2</sub> transitions, respectively. These wavelengths agree with our present values for these lines,  $53.221 \pm 0.005$  Å and  $53.335 \pm 1.005$ 0.005 A. However, it is clear from isoelectronic considerations that most of the intensity of the 53.335-A line is due to the  $3d^{10}4s \, {}^{2}S_{1/2} - 3d^{9}({}^{2}D)4s4p({}^{3}P) \, {}^{4}F_{3/2}^{*}$  transition. Our new value for the  $7p^{2}P_{3/2}^{2}$  level, 1878 940 cm<sup>-1</sup>, is confirmed by observation of the 4d  ${}^{2}D_{5/2}$ -7p  ${}^{2}P_{3/2}^{*}$  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 ----------------- - -

Configuration	Parameter	<b>Y</b> XI	Zr XII	Nb xIII	Mo XIV
$3d9$ 4s4 $p$	A	1 339 595	1529988	1730788	1 241 997
	$G^2(3d4s)$	19 422	20 452	21 479	22 501
	$F^2(3d4p)$	53883	57 598	61 268	64 899
	$G^1(3d4p)$	17428	18610	19 779	20 935
	$G^3(3d4p)$	17 362 <sup>c</sup>	18 605 <sup>a</sup>	19832 <sup>a</sup>	21 046 <sup>a</sup>
	$G^{1}(4s4p)$	93 059	98 402	103703	108 974
	Šаd	6959	8 1 0 3	9376	10787
	Sap	13 128	15770	18741	22 068
$3d^94p^2$	A	1565492	1774993	1994 607	2 2 2 5 0 2
	$F^2(3d4p)$	53 462	57 155	60803	64 413
	$G^{1}(3d4p)$	17404	18 590	19763	20924
	$G^3(3d4p)$	17013	18 236	19444	20 639
	$F^2(4p4p)$	69 351	72864	73 041	75 265
	$\alpha(4p4p)$	$-1017$	$-1017$	$-1017$	$-1017$
	Šза	7 107	8 3 0 2	9638	11 1 25
	ζ4ρ	12 684	15 214	18184	21 435
Configuration Interaction	$R^1(4p4p, 4s4d)$	105857	112 338	118640	124 790

Table 4. Fitted Parameter Values  $(\text{in cm}^{-1})$  for the  $3d^34s4p$  and  $3d^34p^2$ <br>Configurations of  $Y$  at  $Z_2$  and  $Y_1$  and  $Y_2$  and  $Y_3$ **Conf'icurationa** or Y x1, Zr XII, Nb xm, **and Mo** xiv

• **Fiud at** HF value.

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**Table 5. Rartree-Fock Integrals** (in **cm- 1) ror the configurations**  3d<sup>9</sup>4s4p, 3d<sup>9</sup>4p<sup>2</sup>, and 3d<sup>9</sup>4s4d of Y XI, Zr XII, Nb XIII, and Mo XIV

Configuration	<b>Integral</b>	Y xı	$2r \times n$	Nb xIII	Mo XIV
$3d9$ 4s4p	$E_{\rm av}$	1 326 636	1519359	1724 419	1937001
	$G2(3d4s)$ .	19 184	20 20 2	21 216	22 226
	$F^2(3d4p)$	54 307	58 052	61 751	65 410
	$G^1(3d4p)$	17764	18969	20 160	21 339
	G <sup>3</sup> (3d4p)	17 362	18605	19832	21 046
	$G^1(4s4p)$	118 392	124 758	131 028	137 217
	$\zeta_{3d}$	6770	7909	9183	10 600
	5ap	11 668	14 015	16 657	19613
$3d^94p^2$	Eav	1525782	1733 589	1953431	2 181 418
	$F^2(3d4p)$	54 193	57937	61 635	65 294
	$G^{1}(3d4p)$	17698	18 904	20 097	21 277
	$G^3(3d4p)$	17 300	18544	19772	20 987
	$F^2(4p4p)$	89810	94 775	99 675	104 519
	Šаd	6772	7911	9184	10 601
	Š4p	11 640	13985	16 624	19 579
$3d9$ 4s4d	$\bm{E_{\text{ev}}}$	1643121	1862502	2093871	2 332 554
	$F^2(3d4d)$	46 395	50 995	55 546	60 053
	F <sup>4</sup> (3d4d)	21 681	24 038	26 379	28705
	G <sup>0</sup> (3d4d)	15728	17215	18673	20 105
	$G^2(3d4d)$	18 298	20 210	22 099	23 966
	G <sup>4</sup> (3d4d)	13 497	15 457	16954	18438
	$G^2(3d4s)$	19 224	20 230	21 234	22 235
	$G^2(4s4d)$	80 820	86 671	92 274	97 663
	Šза	6780	7920	9 1 9 3	10610
	Šed	1 1 4 7	1 435	1766	2146
Configuration Interaction	$R^1(4p4p, 4s4d)$	110744	117 524	124 116	130 550

as  $\alpha$  and  $\beta$  in Fig. 1. The 7p energy levels are given in Table 8.

# **3d-tp Transitiom in Zn-like and Ni-like Ions**

The remaining satellite lines are the  $3d^{10}4s^2-3d^94s^24p$  tran**sitions** in **the Zn-like** ions. Our identifications for the

 $3d^94s^24p$ <sup>1</sup> $P_1^*$  and  ${}^3D_1^*$  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  $3d^{10}4s^2 \, {\rm^1S_0} - 3d^94s^2 \, 4p \, {\rm^3P_1^*}$ 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

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Table 6. Experimental Levels of  $3d^34p^2$  <sup>o</sup>

<sup>e</sup> The deviations  $\Delta E = E_{\text{exp}} - E_{\text{th}}$  are taken from the generalized least-aquares treatment of the whole sequence. Predicted energies for unknown levels are given in  $LS$  coupling with parent term of  $4p^2$  in parenthe given.

**bLeading component, (3P) <sup>4</sup>F, 49%.<br>
<b>C** Leading component, (3P) <sup>2</sup>D, 40%.

. **<sup>d</sup>Leading** component, (ID) <sup>2</sup>P, 26%.

• **Leading** component, (<sup>3</sup>P) 2P, 47%.

*I* Leading component,  $(3P)$  <sup>4</sup>P, 30%.

• **Leadi111** component, (<sup>3</sup>P) *<sup>4</sup>*F, 29%.

<sup>~</sup>**1-dinc** component, (<sup>3</sup>P) *4*F, 26%.





# Table 8. Energy Levels (in cm<sup>-1</sup>) of the  $3d^{107}p$ **Configurations of Y XI, Zr XII, Nb XIII, and Mo XIV<sup>0</sup>**



• The values in parentheses are derived from blended lines.

Blended with  $3d^{10}4s\sqrt[2]{3}S_{1/2}-3d^24s\sqrt[4]{4}p\sqrt[3]{2}p\sqrt[3]{3}/2p$ .

*b* Blended with  $3d^{10}4s$   $^2S_{1/2}$   $-3d^94s4p$   $(^2D,$  3P)  $^4F_{3/2}$ .



# **Table 9.** *3d-4p* **Transitions** in **Ni-like and Zn-like Ions**

• Blended with  $3p^43d^8$   $^1G_4$ -3p<sup>5</sup>3d<sup>9</sup>  $^1F_3$  transition of Y XIV.

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Table 9. For some lines they differ significantly from the earlier values of Alexander *et al.* <sup>9</sup> Our assignment of the line at  $73.588$  Å as  $3d^{10}$   $^1S_0$   $-3d^94p$   $^3P_1^*$  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 A) **are as** follows (intensities are in parentheses):



**Wyanet** *al.* 

The improved values for Nb XIII **are:** 



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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 A. For Y XIII, Zr XIV, Nb  $xy$ , and Mo  $xy1$  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 Hanree-Fock and least-squares parametric calculations. New wavelengths were obtained for the  $3p<sup>6</sup>3d<sup>9</sup>-3p<sup>5</sup>3d<sup>10</sup>$  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<sup>1</sup> as well as in the DITE tokamak in England.<sup>2</sup> 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 *3p63d9•* The first excited configuration is  $3p<sup>5</sup>3d<sup>10</sup>$ , which gives rise to three strong resonance transitions at relatively long wavelengths (70 A 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 A 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,<sup>3</sup> 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<sup>4</sup>; for Sr XII, Y XIII, and Zr XIV, the wavelengths may also be inferred from the level values given in *Atomic Energy Levels.* <sup>5</sup>In 1971, Alexander *et al.* 6 reported measurements for the 3p63d9-3p53d10 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*8*4p transitions of Sr XII and Y XIII were first observed by Edlen. 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.<sup>6</sup>* published wavelengths with no identifications for about 25 lines of this group in each of the ions from Y XJII to Mo XVI. Mansfield *et al.* <sup>2</sup> 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.*<sup>7</sup> 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<sup>9</sup> 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 A/mm at 60 A. The spectrum of Sr was photographed at an angle of incidence of 80°. The plate factor was 0.17 A/mm. The spectra were excited by means of a low-inductance vacuum spark operating **at a** capacitance of  $14 \mu F$  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 **wave**length 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  $3d^9$  <sup>2</sup>D<sub>5/2</sub>-3d<sup>8</sup>(<sup>3</sup>F)4p <sup>2</sup>F<sub>7/2</sub> transition in each spectrum was given a value of 1000.

The wavelengths, intensities, and classifications of the  $3d^9-3d^64p$  transitions are given in Table 1. The uncertainty of the wavelengths is estimated as  $\pm 0.005$  A. The present values for the  $3p^{6}3d^{9}-3p^{5}3d^{10}$  transitions are given in Table

Table 1. 3d<sup>9</sup>-3d<sup>8</sup>4p Transitions in Sr XII, Y XIII, Zr XIV, Nb XV, and Mo XVI



 $\degree$  Calculated from fitted values of energy parameters.<br>  $\degree$  Present value for line given by Burkhalter *et al.*, Ref. 7.<br>  $\degree$  Doubly classified.<br>  $\degree$  Doubly classified.<br>  $\degree$  Present value for line given by Burkhalte

2, along with the values previously reported. The present **SPECTRUM ANALYSIS** values for Sr XII are not compared with those of Ref. 8 because the measurements were taken from the same exposures and the measurements were taken from the same exposures and The observations were interpreted by comparing the observed

spectra with calculated wavelengths and intensities of the five

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# $\begin{bmatrix} . & . & . \\ . & . & . \\ . & . & . \\ . & . & . & . \end{bmatrix}$ <br>
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Table 2. 3p<sup>6</sup>3d<sup>9</sup>-3p<sup>5</sup>3d<sup>10</sup> Transitions in Sr XII, Y XIII, Zr XIV, Nb XV, and Mo XVI



<sup>e</sup> This work.<br>• Alexander *et al*., Ref. 6.<br>• Burkhalter *et al.*, Ref. 7.





<sup>a</sup> Values for unobserved levels, given in parentheses, are those calculated with the fitted values of the energy parameters.

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ions. The calculations were made with a set of computer codes developed by the Institute of Physics of the Lithuanian Academy of Sciences.<sup>15,16</sup> The radial integrals were first computed by a Hartree-Fock (HF) calculation and then scaled by factors obtained by extrapolation along the Co 1 isoelectronic sequence.<sup>17,18</sup>

Although **the observed spectra are** complex and blended in some regions, the predicted isoelectronic trends yielded un-





Table 4. Spin-Orbit Parameters  $\zeta_{3d}$  (in cm<sup>-1</sup>) for the **3p<sup>6</sup>3d9 Configurations of Sr XII, Y XIII, Zr** XIV, **Nb** XV, and Mo XVI

HF	Obs.	Obs./HF
5836	5864	1.005
6863	6892	1.004
8016	8056	1.005
9 3 0 4	9 3 5 2	1.005
10737	10808	1.007

**Table 5. Energy Parameters (in cm-1) for the 3p<sup>5</sup>3d<sup>10</sup> Configurations of Sr XII, y XIII, Zr XIV, Nb xv, and Moxv1** 



Table 6. Energy Parameters and Mean Errors  $\Delta$  (in **cm- 1) for the** *3d"4p* **Configurations of Sr xu, Y XIII,**  Zr XIV, Nb xv, and Mo XVI

	Param-			
Ion	eter	HF	<b>Fitted</b>	<b>Fitted/HF</b>
<b>Sr xii</b>	$E_{av}$	1 356 870	$1340470 \pm$ 130	
	$F^2(3d3d)$	214 010	192 820 ± 910	$0.901 \pm 0.004$
	F <sup>4</sup> (3d3d)	136 318	$116630 \pm 3480$	$0.856 \pm 0.026$
	$\alpha_1(3d3d)$		$107 \pm$ 40	
	$F^2(3d4p)$	55 593	$54830 \pm$ 930	$0.986 \pm 0.017$
				$0.974 \pm 0.019$
	$G^1(3d4p)$	18218	$17740 \pm$ 340	
	$G^3(3d4p)$	17886	$20560 \pm 2040$	$1.150 \pm 0.114$
	$\alpha(3d4p)$		$69 \pm$ 56	
	$\zeta_{3d}$	6088	$6180 +$ 90	$1.015 \pm 0.015$
	Š4р	11 329	$12540 \pm$ 230	$1.107 \pm 0.020$
	Δ		200	
Y XIII	$E_{av}$	1 551 260	$1530440 \pm$ 70	
	$F^2(3d3d)$	224 667	$204370 \pm$ 610	$0.910 \pm 0.003$
	F <sup>4</sup> (3d3d)	143 263	$130100 \pm$ 520	$0.908 \pm 0.004$
	$\alpha_1(3d3d)$		24 $71 \pm$	
	$F^2(3d4p)$	59 275	60 220 $\pm$ 530	$1.016 \pm 0.009$
	$G^1(3d4p)$	19 399	$19210 \pm$ 230	$0.990 \pm 0.012$
	$G^3(3d4p)$	19 106	$20800 \pm 1090$	$1.089 \pm 0.057$
			$32 \pm$ 22	
	$\alpha(3d4p)$			
	53d	7144	$7180 \pm$ 70	$1.005 \pm 0.010$
	$\zeta_{4p}$	13586	120 $15150 \pm$	$1.115 \pm 0.009$
	Δ		240	
Zr XIV	$E_{av}$	1755480	$1731230 \pm$ 60	
	$F^2(3d3d)$	235 264	$214890 \pm$ 580	$0.913 \pm 0.002$
	F <sup>4</sup> (3d3d)	150 169	480 $136350 \pm$	$0.908 \pm 0.003$
	$\alpha_1(3d3d)$		24 $76 \pm$	
	$F^2(3d4p)$	62917	450 63 970 $\pm$	$1.017 \pm 0.007$
	$G^{1}(3d4p)$	20 569	220 $20360 \pm$	$0.990 \pm 0.011$
	$G^3(3d4p)$	20 312	$22150 \pm 1170$	$1.090 \pm 0.058$
	$\alpha(3d4p)$		23 $34 \pm$	
	$\zeta_{3d}$	8328	$8410 \pm$ 70	$1.010 \pm 0.008$
		16 127	$17910 \pm$ 110	$1.111 \pm 0.007$
	$\zeta_{4p}$ Δ		240	
Nb xv	$E_{av}$	1972210	$1942790 \pm$ 70	
	$F^2(3d3d)$	245 805	$226020 \pm$ 740	$0.920 \pm 0.003$
	F <sup>4</sup> (3d3d)	157 039	$143220 \pm$ 610	$0.912 \pm 0.004$
	$\alpha_1(3d3d)$		$66 \pm$ 28	
	$F^2(3d4p)$	.66 526	67 860 ± 640	$1.020 \pm 0.010$
	G <sup>1</sup> (3d4p)	21 729	$21630 \pm$ 260	$0.995 \pm 0.012$
	$G^3(3d4p)$	21 507	$22950 \pm 1490$	$1.067 \pm 0.069$
	$\alpha(3d4p)$		27 45±	
	$\zeta_{3d}$	9650	$9690 \pm$ 70	$1.004 \pm 0.007$
	Š4ρ	18974	$21120 \pm$ 130	$1.113 \pm 0.007$
	Δ		270	
		2 198 910		
<b>Mo XVI</b>	$E_{av}$ $F^2(3d3d)$	256 302	$2165110 \pm$ 80 $235430 \pm$ 760	$0.919 \pm 0.003$
	$F^4(3d3d)$	163 880	$149560 \pm$ 650	$0.913 \pm 0.004$
	$\alpha_1(3d3d)$		27 $51 \pm$	
	$F^2(3d4p)$	70 106	$71150 \pm 660$	$1.015 \pm 0.009$
	$G^1(3d4p)$	22 879	$22810 \pm$ 250	$0.997 \pm 0.011$
	$G^3(3d4p)$	22 692	$23710 \pm 1550$	$1.045 \pm 0.068$
	$\alpha(3d4p)$		27 $51 \pm$	
	Sad	11 119	$11180 \pm$ 70	$1.005 \pm 0.006$
	Š4р	22 150	$24690 \pm$ 130	$1.115 \pm 0.006$
	Δ		270	

ambiguous 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  $32$ 

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stages. The identifications are supported by repetititon of the 3d9 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 *3d9* <sup>2</sup>D 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  $3d^{9}$   ${}^{2}D_{5/2}$   $-3d^{8}$ ( ${}^{3}F$ ) $4p$   ${}^{2}D_{5/2}$  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*<sup>8</sup>*4p* levels relative to the ground term is approximately  $\pm 200$  cm<sup>-1</sup>. The relative values within  $3d^{8}4p$  are uncertain by about  $\pm 100 \text{ cm}^{-1}$ . The 3d<sup>9</sup> <sup>2</sup>D intervals were derived from all observed pairs, with double weight given to the  $3p^63d^9$  ${}^{2}D_{5/2,3/2}$  ${}^{3}D^{5}3d^{10}$   ${}^{2}P_{3/2}$  pair because of its longer wave-length.

The structure of the  $3d^84p$  configuration of  $Zr$  XIV is shown in Fig. 1. Although the levels are designated in the *LS-cou*pling 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 iaoelectronic 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 3d84p Configurations of Sr XII, Zr XIV, and Mo XVI

J	Term	Percent $J_1j$	Percentage Composition (LS)
1/2	$(^3F)^4D$	$73,62,48\%$ ( ${}^{3}F_{2}$ , $3/2$ )	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% $({}^{3}P)^{4}P + 5$ , 4, 2% $({}^{1}D)^{2}P + 2$ , 3, 5% $({}^{3}P)^{4}D$
	$(^3P)^4D$	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% $(1D)$ <sup>2</sup> P + 32, 19, 31% $(3P)$ <sup>2</sup> P + 11, 2, 17% $(3F)$ <sup>4</sup> D
	$(3P)$ <sup>2</sup> S	66, 66, 68% $(3P_1, 3/2)$	57, 61, 61% $({}^{3}P)^{2}S + 27$ , 22, 19% $({}^{3}P)^{2}P + 6$ , 7, 8% $({}^{3}P)^{4}D$
	$(3P)$ <sup>2</sup> $P$	60, 53, 47% $(^{3}P_{2}$ , 3/2)	33, 33, 34% $({}^{3}P){}^{2}P + 32$ , 24, 19% $({}^{3}P){}^{2}S + 30$ , 35, 38% $({}^{1}D){}^{2}P$
	$(^{1}S)^{2}P$	93, 91, 88% $(^1S_0$ , 1/2)	93, 91, 88% $(^{1}S)^{2}P + 3$ , 3, 4% $(^{1}D)^{2}P + 2$ , 3, 4% $(^{3}P)^{4}D$
3/2	$(^3F)^4F$	60, 55, 42% $(^3F_2, 1/2)$	27, 26, 20% $({}^{3}F){}^{4}F + 37$ , 14, 6% $({}^{3}F){}^{4}D + 10$ , 21, 26% $({}^{1}D){}^{2}D$
	$(^3F)^4D$	35, 39, 31% $(^3F_3$ , 3/2)	40, 54, 50% $({}^{3}F)^{4}D + 13$ , 20, 24% $({}^{3}P)^{4}D + 7$ , 10, 13% $({}^{3}P)^{4}P$
	(3P)4P	38, 38, 30% ( <sup>3</sup> P <sub>2</sub> , 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% $({}^{3}F)^{2}D + 31$ , 41, 40% $({}^{3}F)^{4}F + 23$ , 15, 14% $({}^{3}P)^{4}P$
	$(1D)$ <sup>2</sup> D	31, 13, 2% $(^1D_2, 1/2)$	$31, 20, 11\%$ ( ${}^{1}D$ ) ${}^{2}D + 29, 22, 15\%$ ( ${}^{3}F$ ) ${}^{2}D + 12, 22, 28\%$ ( ${}^{3}P$ ) ${}^{2}P$
	$(^3P)^4D$	66, 37, 17% $(3P_1, 1/2)$	50, 29, 14% $({}^{3}P)^{4}D + 6$ , 20, 36% $({}^{3}F)^{2}D + 6$ , 15, 21% $({}^{1}D)^{2}D$
	$(1D)$ <sup>2</sup> $P$	75, 57, 35% $(^{1}D_{2}, 3/2)$ .	61, 53, 38% $(1D)$ <sup>2</sup> P + 19, 11, 5% $(1D)$ <sup>2</sup> D + 3, 9, 17% $(3P)$ <sup>2</sup> P
	$(3P)$ <sup>2</sup> $P$	48, 34, 17% $(3P_2, 3/2)$	65, 52, 37% $({}^{3}P)^{2}P + 10$ , 16, 17% $({}^{1}D)^{2}D + 10$ , 13, 15% $({}^{3}P)^{4}D$
	$(^3P)^2D$	50, 45, 33% $(^3P_0, 3/2)$	78, 74, 69% $({}^{3}P)^{2}D + 12$ , 12, 9% $({}^{3}P)^{4}D + 3$ , 4, 5% $({}^{1}S)^{2}P$
	$(3P)^4S$	47, 47, 47% $(3P_1, 3/2)$	87, 82, 75% $(3P)^4S + 4$ , 5, 8% $(3P)^2P + 3$ , 4, 3% $(3P)^4P$
	$(1S)$ <sup>2</sup> $P$	$95, 93, 91\%$ ( $^{1}S_0, 3/2$ )	$-95.93.91\%$ $(1S)^2P + 2.2.2\%$ $(1D)^2P + 1.2.2\%$ $(3P)^2D$
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% $({}^3F)^4F$
	$(^3F)^2D$	$30, 29, 25\%$ ( ${}^{3}F_{4}$ , $3/2$ )	48, 46, 41% $({}^{3}F){}^{2}D + 18$ , 22, 26% $({}^{3}F){}^{4}G + 16$ , 11, 7% $({}^{3}F){}^{4}F$
	$(3F)^4F$	65, 69, 66% $(^3F_3$ , 3/2)	37, 35, 33% $({}^{3}F){}^{4}F + 21$ , 19, 16% $({}^{3}F){}^{2}F + 14$ , 19, 19% $({}^{3}F){}^{4}D$
	(3P)4P	28, 31, 29% $(^3P_2, 1/2)$	$31, 27, 20\%$ ( <sup>3</sup> P) <sup>4</sup> P + 22, 29, 32% ( <sup>3</sup> F) <sup>2</sup> D + 14, 11, 10% ( <sup>1</sup> D) <sup>2</sup> F
	$(^3F)^2F$	48, 33, 21% $(^3F_2$ , 3/2)	54, 43, 36% $({}^{3}F){}^{2}F + 15$ , 17, 15% $({}^{1}D){}^{2}F + 6$ , 13, 18% $({}^{1}D){}^{2}D$
	$(1D)$ <sup>2</sup> $F$	$31, 31, 34\%$ ( $^{1}D_{2}$ , $1/2$ )	35, 26, 22% $(1D)$ <sup>2</sup> F + 45, 38, 28% $(3P)$ <sup>4</sup> P + 8, 11, 13% $(3F)$ <sup>4</sup> G
	(1D)2D	$9, 17, 25\%$ $(^3P_2, 3/2)$	36, 21, 9% $(1D)^2D + 29$ , 29, 24% $(3P)^2D + 11$ , 18, 26% $(3F)^2F$
	$(^3P)^4D$	$32, 33, 28\%$ ( $^{1}D_{2}$ , $3/2$ )	24, 17, 14% $({}^{3}P)^{4}D + 23$ , 27, 24% $({}^{1}D)^{2}D + 14$ , 22, 30% $({}^{1}G)^{2}F$
	$(^3P)^2D$	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% ( ${}^{1}G_{4}$ , 3/2)	63, 53, 43% $(^1G)^2F$ + 7, 11, 16% $(^1D)^2D$ + 10, 11, 11% $(^1D)^2F$
7/2	$(^3F)^4D$	$87, 89, 91\%$ ( ${}^{3}F_{4}$ , $1/2$ )	77, 73, 69% $({}^{3}F){}^{4}D + 13$ , 15, 16% $({}^{3}F){}^{4}F + 5$ , 6, 8% $({}^{3}F){}^{2}F$
	$($ <sup>3</sup> $F$ ) <sup>4</sup> $G$	$87, 89, 91\%$ ( ${}^{3}F_{3}$ , $1/2$ )	68, 66, 65% ( ${}^{3}F$ ) <sup>4</sup> G + 13, 14, 15% ( ${}^{3}F$ ) <sup>2</sup> G + 14, 12, 12% ( ${}^{3}F$ ) <sup>4</sup> F
	$(3F)$ <sup>2</sup> $F$	67.74.79% $(3F4, 3/2)$	53, 57, 59% $(3F)$ <sup>2</sup> F + 25, 20, 15% $(3F)$ <sup>4</sup> F + 12, 15, 18% $(3F)$ <sup>4</sup> D
	$(^3F)^4F$	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% ( ${}^{1}G_{4}$ , 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) <sup>4</sup> D + 43, 26, 8% ( <sup>1</sup> G) <sup>2</sup> F + 1, 5, 14% ( <sup>3</sup> F) <sup>2</sup> G
	$(1D)^2F$	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% ( ${}^{3}F$ ) <sup>4</sup> G + 33, 36, 37% ( ${}^{3}F$ ) <sup>2</sup> G + 24, 23, 23% ( ${}^{3}F$ ) <sup>4</sup> F
	$(^3F)^4F$	$97, 98, 98\%$ ( ${}^3F_4$ , 3/2)	71, 71, 70% $({}^{3}F){}^{4}F + 23$ , 25, 26% $({}^{3}F){}^{2}G + 5$ , 3, 2% $({}^{3}F){}^{4}G$
	$(^3F)^2G$	$96, 98, 99\%$ ( $^{3}F_{3}$ , $3/2$ )	43, 37, 34% $({}^{3}F)^{2}G + 53$ , 57, 60% $({}^{3}F)^{4}G + 4$ , 5, 6% $({}^{3}F)^{4}F$
	$(^{1}G)^{2}H$	$92, 93, 94\%$ ( ${}^{1}G_{4}$ , 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	$(^3F)^4G$	$99, 99, 98\%$ ( ${}^{3}F_{4}$ , $3/2$ )	99, 99, 98% $(^3F)^4G + 1$ , 1, 2% $(^1G)^2H$
	$(^1G)$ <sup>2</sup> H	99, 99, 98% $(^{1}G_{4}, 3/2)$	99, 99, 98% $(^1G)^2H + 1$ , 1, 2% $(^3F)^4G$

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

<b>Level Designation</b>	<b>Percentage Composition</b>	
$(^1D)^2P_{1/2}$	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% ( ${}^{3}P$ ) <sup>4</sup> D + 11, 30, 0, 5, 12% ( ${}^{1}D$ ) <sup>2</sup> P + 12, 5, 31, 28, 26% ( ${}^{3}F$ ) <sup>4</sup> D + 3, 7, 0, 2, 5% ( ${}^{3}P$ ) <sup>2</sup> S $+2, 4, 0, 0, 0\%$ (3P) <sup>4</sup> P + 2, 1, 17, 8, 4% (3P) <sup>2</sup> P + 1, 0, 4, 3, 3% (1S) <sup>2</sup> P	

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  $\zeta_{3d}$  for the  $3d^9$  configuration with those calculated with the HF program of Froese-Fischer.<sup>19</sup> In Table 5 we give a similar comparison for the  $3p<sup>5</sup>3d<sup>10</sup>$  configuration.

In Table 6 the values of the energy parameters obtained at NBS from least-squares fits to the observed  $3d<sup>8</sup>4p$  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  $3d<sup>8</sup>$  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<sup>8</sup> 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  $J_{1}j$  and the *J 1l* schemes are similarly low. The values.of unobserved  $3d<sup>8</sup>4p$  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<sup>9</sup> 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  $3d^9$ <sup>2</sup> $D_{3/2}$  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 A on the average. Considering that the wavelength uncertainty of Burkhalter *et al.* <sup>7</sup> was  $\pm 0.010$  Å and that our present uncertainty is  $\pm 0.005$  Å, the wavelengths are in satisfactory agreement. Five of the Mo XVI lines in Table 1 were not observed by Burkhalter *et* al.<sup>7</sup> 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.<sup>9</sup> In the Co sequence  $\alpha_1(3d3d)$  has its maximum value<sup>17,18</sup> at about Kr X. This may be the consequence of a perturbation of the  $3p<sup>6</sup>3d<sup>8</sup>4p$  configuration by  $3p<sup>5</sup>3d<sup>10</sup>$ , 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  $3p^{5}3d^{10}$  <sup>2</sup>P<sub>3/2</sub>, and we therefore omitted it from the leastsquares 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  $({}^{3}P){}^{4}D_{1/2}$  and  $({}^{1}D){}^{2}P_{1/2}$  levels. The  $({}^{3}P){}^{4}D_{1/2}$  level is calculated to lie above  $({}^{1}D){}^{2}P_{1/2}$  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<sup>6</sup>3d<sup>8</sup> <sup>1</sup>S<sub>0</sub> level of Sr XIII, Y XIV, Zr** *XV***, Nb** *XVI***, and** Mo **xv**II

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# Received March 12. 1983

Following an observation by Wyart *et al.* [Phys. Scr. 26, 141 (1982)], we have revised the position of the 3p<sup>6</sup>3d<sup>81</sup>S<sub>0</sub> level in Sr XIII, Y XIV, Zr XV, Nb XVI, and Mo XVII and have redetermined the 3 $p^{\rm 63d^{\rm 8}}$  energy parameters in these ions.

Recently, Reader and Ryabtsev<sup>1</sup> analyzed the  $3p^63d^8$ - $3p<sup>5</sup>3d<sup>9</sup>$  transitions in the isoelectronic ions Sr XIII-Mo XVII. In this analysis the  $3p^63d^8$ <sup>1</sup>S<sub>0</sub> level was established by the single transition  $3p^63d^8$   $^1S_0$ - $3p^53d^9$   $^1P_1$ . Subsequently, 3p63d9-3p63d84p transitions were analyzed in Sr XII-Mo XVI by Ryabtsev and Reader2 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  $3p^63d^8$  <sup>1</sup>S<sub>0</sub> level for the ions Sr XIII-Nb XVI in Ref. 1. Further, they proposed new identifications for the  $3p^63d^8$   ${}^{1}S_0$ - $3p^53d^9$   ${}^{1}P_1$  transitions in Y XIII-Nb XVI.

We have reviewed our spectra .: this regard and have found transitions of the type  $3p^63d^8$ <sup>1</sup>S<sub>0</sub>-3p<sup>5</sup>3d<sup>9</sup><sup>3</sup>D<sub>1</sub> that support the proposed identifications of Wyart *et al.*<sup>3</sup> A 3p<sup>6</sup>3d<sup>8</sup>  $1S_0-3p^53d^9$   $^3D_1$  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  $3p^{6}3d^{8}$  configuration we have also revised the  $3p^63d^8$   ${}^{1}S_0$ -3 $p^53d^9$   ${}^{1}P_1$  identification in Sr XIII. The lines identified as  $3p^63d^8$   $^1S_0$ -3 $p^53d^9$   $^1P_1$ 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 man**ganeselike** ions.•

In Table 1 we give the  $3p^{6}3d^{8}$ <sup>1</sup>S<sub>0</sub>-3p<sup>5</sup>3d<sup>9</sup><sup>1</sup>P<sub>1</sub> and 3p<sup>6</sup>3d<sup>8</sup>  $1S_0-3p^63d^{9}$   $3D_1$  transitions in the ions Sr XIII-Mo XVII. The revised positions of the  $3p^63d^8$  <sup>1</sup>S<sub>0</sub> level in these ions are given in Table 2. The revision of  $3p^63d^8$  <sup>1</sup>S<sub>0</sub> 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  $3p^63d^8$  <sup>1</sup>S<sub>0</sub> 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<sup>1</sup> 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 previously1 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 thoee of Ref. 1 and are therefore not given here.

# ACKNOWLEDGMENT

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• Intensities **are viauaJ estimates** of photographic blackening.

<sup>b</sup> Blended with  $4p$  <sup>2</sup>P<sub>3/2</sub>-6s <sup>2</sup>S<sub>1/2</sub> transition of Nb XIII.

# **Table 2.**  $3p^63d^8$  <sup>1</sup> $S_6$  Levels of Sr XIII-Mo XVII  $(in cm^{-1})$



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# Table 3. Energy Parameters (in cm<sup>-1</sup>) and Mean Errors  $\Delta$  of Least-Squares Fits for the  $3p^43d^8$  Configurations of Sr XIII, Y XIV, Zr XV, Nb XVI, and Mo XVII<sup>a</sup>

<sup>0</sup>The value for£,. listed in the HF column is that obtained by diagonalizing the energy **matrix** with the HF **parameters,** <sup>3</sup>F, 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<sup>6</sup>3d<sup>8</sup> Configurations of Sr XIII, Y XIV, Zr XV, Nb XVI, and **Moxvn** 



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**ATTACHMENT** 

# 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<br>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.

# Artic1e 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.  $n$ hich 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, scien**tific** 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 infonn 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 infonn 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 ~cientists 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 shaTl 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 Executiva Agents designated in Article VIl 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 £nglish and Russian languages, both equally authentic. -

For the US National Bureau of Standards

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.Director

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For the USSR Academy of Sciences

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