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ABSTRACTS & PROGRAM

SAS-83

Symposium on Atomic Spectroscopy

Lawrence Berkeley Laboratory
University of California
Berkeley, CA 94720

September 1983

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**Symposium on Atomic Spectroscopy
(SAS-83)**

September 12-16, 1983

**Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720**

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Symposium on Atomic Spectroscopy
(SAS-83)
September 12-16, 1983
Berkeley, California

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PROGRAM

Monday, September 12

8:00 a.m. Registration in main lobby of
Shattuck Hotel

All events will take place in
main ballroom.

Rydbergs, Optical Radiators, and Planetary Atoms

9:00 a.m. Welcoming Remarks: David A. Shirley, LBL Director

9:15 a.m. E. Matthias (Joint Institute for Laboratory
Astrophysics & National Bureau of Standards)

*Hyperfine Structure as a Probe of State
Mixing in Rydberg, States of Alkaline-Earth Atoms*

9:45 a.m. Michael S. Feld (Massachusetts Institute of Technology)

*Observation of Quantum Diffractive Collisions
Using Two Level Heavy Optical Radiators*

10:15-10:40 a.m. Coffee Break

10:45 a.m. R.R. Freeman (Bell Laboratories)

Planetary Atoms

11:15 a.m. R. Beach, B. Brody, M. Glick, P. Yang, and S.R. Hartmann
(Columbia Radiation Laboratory)

Angled Beam Photon Echoes

11:30 a.m. W.R.S. Garton, J.P. Connerade, T.A. Stavrakas (Imperial College)

J. Hormes, M.A. Baig, B. Alexa (Physikalishes Institut, Bonn)

H.M. Crosswhite, H. Crosswhite, and F.S. Tomkins

(Argonne National Laboratory)

Zeeman Spectra of Rydberg Series

11:45 a.m. V. Kaufman, J. Sugar, C.W. Clark, and W.T. Hill, III
(National Bureau of Standards)

*Rydberg Series $5p^56sns$ and $5p^56snd$ in the
Autoionizing Continua of Neutral Cesium*

12:00-1:50 p.m. Lunch

Highly Ionized

Thomas Gallager, Presiding

- 2:00 p.m. Brian C. Fawcett (Rutherford Appleton Laboratory)
Spectroscopy of Highly Ionized Atoms
- 2:30 p.m. Jean Blaise (Laboratoire Aimé Cotton)
Spectroscopy of the Neutral and Singly Ionized Actinides
- 3:00-3:25 p.m. Coffee Break
- 3:30 p.m. J.O. Ekberg (University of Lund)
Extended Analysis of Fe III in the Vacuum Ultraviolet
- 3:45 p.m. Torkild Andersen (University of Aarhus),
Jørgen E. Hansen (Zeeman Laboratory), Willy Persson and
Sven-Eiöran Pettersson (Lund Institute of Technology)
*Identification of the $ns^0np^6\ ^1S_0$
Level of Ar III and Kr III by Optical Spectroscopy*
- 4:00 p.m. V. Kaufman and J. Sugar (National Bureau of Standards)
The $4d^95s5p$ Configuration in I VII through Eu XVII
- 4:15 p.m. Rolf Engleman, Jr. and Bryon A. Palmer
(Los Alamos National Laboratory)
The Atomic Spectrum of Neutral Gold
- 4:30 p.m. L. Iglesias, F.R. Rico, O. García-Riquelme
(Instituto de Optica, Serrano)
V. Kaufman (National Bureau of Standards)
The Spectrum of Doubly Ionized Tungsten, W III
- 6:00-8:00 p.m. Reception at the Alumni House of the
University of California

Ultraviolet

Harry White, Presiding

Tuesday, September 13

- 8:00 a.m. Registration in main lobby of Shattuck Hotel
- 9:00 a.m. Bernd Crasemann (University of Oregon)
Atomic Inner-Shell Transitions
- 9:30 a.m. R.C. Elton (Naval Research Laboratory)
Spectroscopy of X-Ray Lasers
- 10:00-10:25 a.m. Coffee Break
- 10:30 a.m. S.E. Harris (Edward L. Ginzton Lab., Stanford University)
Laser Spectroscopy in the Extreme Ultraviolet
- 11:00 a.m. Wojciech Gawlik, (Uniwersytet Jagielloński)
Joachim Kowalski, Frank Träger, and Michael Vollmer
(Universität Heidelberg)
Subnatural Linewidth Effects in Polarization Spectroscopy
- 11:15 a.m. J. Kowalski, G. zu Putlitz, F. Träger, and M. Vollmer
(Universität Heidelberg)
*Method for Signal Enhancement in Laser Spectroscopy of
Metastable States*
- 11:30 a.m. C. Karner, M. Milicev, R. Neumann, F. Träger and
G. zu Putlitz (Universität Heidelberg)
Ultraviolet Laser Spectroscopy of Doubly Charged Europium Ions
- 12:00-1:50 p.m. Lunch
- 2:00-4:30 p.m. POSTER SESSION
1. James W. Brault (Kitt Peak National Observatory)
*First and Second Spectra of Transition and Light
Metals in the 1-5.5 Micron Region by Fourier
Spectroscopy*
 2. Ward Whaling (California Institute of Technology)
*Atomic Level Populations in the Hollow Cathode
Spectral Light Source*

3. Joseph Reader, Nicolo Acquista, and David Copper
(National Bureau of Standards)
*Laser-Produced Spectra of Copperlike Ions from
Ru¹⁵⁺ to Sn²¹⁺*
4. Craig J. Sansonetti and W.C. Martin
(National Bureau of Standards)
*Accurate Wavenumber Measurements for the ⁴He I
1s2p-1s3d Transitions*
5. W.C. Martin, J. Sugar, J. Reader, and A. Albright
(National Bureau of Standards)
Compilations of Atomic Energy Levels
6. G.A. Martin, J.R. Fuhr, and W.L. Wiese
(National Bureau of Standards)
Critical Complications of Atomic Transition Probabilities
7. D.D. Dietrich, R.J. Fortner, and R.E. Stewart
(Lawrence Livermore National Laboratory)
R.J. Dukart (Physics International)
*Wavelength Measurements of 2s-2p Transitions in Fluorinelike
and Oxygenlike Krypton XXVIII and XXIX*
8. D.D. Dietrich, C.J. Hailey, G.A. Chandler,
M.J. Eckart, R.E. Stewart and R.J. Fortner
(Lawrence Livermore National Laboratory)
*New Technique for X-Ray Line Measurements in Fast
Ion Spectroscopy*
9. Mireille Aymar, (Laboratoire-Aimé Cotton)
*Rydberg Levels of Alkaline-Earth Spectra: MQDT
Wavefunctions Probed by Laser Measurements*
10. Byron A. Palmer and Rolf Engleman, Jr.
(Los Alamos National Laboratory)
The Third Spectra of Uranium and Thorium
11. R.E. Stewart, D.D. Dietrich, R.J. Fortner, and M.J. Eckart
(Lawrence Livermore National Laboratory)
*Detailed Analysis of 4-2, 3-2, and 3-3 Emission Spectra
from Neon-like and Near Neon-like Krypton Produced in
a Z-Pinch Plasma*

Theory

Wednesday, September 14

- 9:00 a.m. B.R. Judd (The Johns Hopkins University)
Theoretical Procedures for Atomic Energy Levels
- 9:30 a.m. Charlotte Froese Fischer (Vanderbilt University)
Computational Spectroscopy
- 10:00-10:25 a.m. Coffee Break
- 10:30 a.m. H.M. Crosswhite and H. Crosswhite
(Argonne National Laboratory)
Parametric Fitting for Low Odd Configurations of U II
- 10:45 a.m. B.R. Judd (The Johns Hopkins University), J.E. Hansen
(Zeeman Laboratory)
*Parametric Fitting to the p^nd Configurations Using
a Complete Set of Two- and Three-Body Parameters*
- 11:00 a.m. R.M. Sternheimer (Brookhaven National Laboratory)
Possible Implications of the k Ordering of Atomic Structure
- 11:15 a.m. Zipora B. Goldschmidt (Hebrew University of Jerusalem)
*Matrix Elements for Spin-Dependent Interactions in l^Nl'
Configurations*
- 12:00-1:50 p.m. Lunch

Theory, Ion Traps, and Laser Cooling

Joseph Reader, Presiding

- 2:00 p.m. Harvey Gould (Lawrence Berkeley Laboratory)
ArII-ArXVI Produced in Slow Recoil Collisions
- 2:15 p.m. R. Blatt, W. Ertmer, and J.L. Hall (University of Colorado
and National Bureau of Standards)
Laser Cooling of an Atomic Beam with Frequency-Sweep Techniques

- 2:30 p.m. Dave Wineland (National Bureau of Standards)
Laser Cooling and Ion Frequency Standards
- 3:00-3:25 p.m. Coffee Break
- 3:30 p.m. M.H. Prior (Lawrence Berkeley Laboratory)
Forbidden Spectra and Decay Rates from Metastable Trapped Ions
- 4:00 p.m. Z.B. Goldschmidt, A. Edwards, and O. Hagug
(Hebrew University of Jerusalem)
*Two- and Three-Electron Effective Electrostatic Interactions
in the $3d^N 4p$ Configurations of the Third and Fourth
Spectra of the Iron Group*
- 4:15 p.m. Z.B. Goldschmidt and Z. Vardi
(Hebrew University of Jerusalem)
*Spin-Dependent Interactions in the $3d^N$ Configurations
of the Fourth and Fifth Spectra of the Iron Group*
- 4:30 p.m. Th.A.M. van Kleef, P. Uylings, A.N. Ryabtsev, and Y.N. Joshi
(Universiteit van Amsterdam)
*Configuration Interactions in the Fe I and Co I Sequences
in the Ions of the Elements As, Se and Br*
- Banquet at Lawrence Hall of Science.
Buses depart from the hotel at 5:30 p.m.
and will return to the hotel after the banquet.
- 6:00 p.m. Reception
- 7:00 p.m. Dinner and Speaker

Beam Foil

Raymond Kelly, Presiding

Thursday, September 15

- 9:00 a.m. Ove Poulsen, (University of Aarhus)
Beam Foil Spectroscopy

- 9:30 a.m. A.E. Livingston (University of Notre Dame)
Fast-Ion Spectroscopy of Highly Ionized Atoms
- 10:00-10:25 a.m. Coffee Break
- 10:30 a.m. H.-D. Kronfeldt, J.-R. Kropp, and R. Winkler
(Technischen Universität Berlin)
Application of the Parametric Description of the Isotope Shift (PADIS) to the Lanthanides
- 10:45 a.m. Bruce V. Pulliam (5816 Agawam Dr., Indianapolis, Indiana)
The Use of Hyperfine Structures in the Analysis of the Americium I Spectrum
- 11:00 a.m. S. Büttgenbach and F. Träber
(Universität der Bonn)
Configuration Interaction in the Hyperfine Structure of Transition Elements
- 11:15 a.m. J. Kowalski, R. Neumann, S. Nochte, H. Suhr, and G. zu Putlitz (Universität der Heidelberg)
Effects of Nuclear Structure in the $1s2s\ ^3S_1$ Hyperfine Splittings of Helium-Like $^{6,7}\text{Li}^+$ Ions
- 11:30 a.m. S. Bashkin, K. Brand, H. v. Buttlar, P.H. Heckmann, and E. Träbert (Ruhr-Universität)
Beam-Foil Study of Titanium in the EUV and Population of Yrast Levels
- 12:00-1:50 p.m. Lunch
- 2:00-4:30 p.m. POSTER SESSION
1. E. Biémont (Université de Liège) and G.E. Bromage (Rutherford Appleton Laboratory)
Transition Probabilities for Forbidden Lines: The Silicon Isoelectronic Sequence from S III to Sn XXXVII
 2. Leo Brewer (Lawrence Berkeley Laboratory)
The Need for Complete Assignments of All Low-Lying Atomic Levels for Thermodynamic Calculations
 3. David R. Wood and Jaffer A. Hussainee (Wright State University)
Conversion of a Plane Grating Spectrometer into a Concave Grating Spectrometer for the Far Ultraviolet

4. A. Lucas and R. Winkler (Technische Universität Berlin)
On the Dependency of the Free Spectral Range of a Fabry-Perot-Interferometer on Mirror-Design, Wavenumber and Scanning-Pressure
5. G.O. Brink and S.M. Heider (State University of New York)
Dye Laser Intracavity Absorption for Atomic Absorption Spectroscopy
6. Stephen B. Sears and Frederick H. Mies
(National Bureau of Standards)
Elastic Electron Scattering from Atomic Ions: A Pseudopotential Approach
7. H.G. Berry, D. Neek, L.P. Somerville, and J. Hardis
(Argonne National Laboratory)
100% Alignment of Hydrogen Excited States in Beam-Foil Spectroscopy
8. B. Denne, E. Hinnov, S. Suckewer, and J. Timberlake
(Princeton University)
On the Ground Configuration of the Phosphorous Sequence from Copper to Molybdenum
9. H.A. Klein, F. Moscatelli, and J.D. Silver (Clarendon Laboratory)
N.J. Peacock (Culham Laboratory),
M.F. Stamp (Clarendon Laboratory and Culham Laboratory)
Measurements of $1s2s\ ^3S - as2p\ ^3P$ Transition Wavelengths in Helium-like Ions in the Range $Z = 7$ to $Z = 13$
10. Zhiwen Wang, R-G. Wang, and K.T. Lu
(Argonne National Laboratory)
Graphic Analysis of Open-Shell Atom-Chlorine
11. J.P. Buchet, M.C. Buchet-Poulizac, A. Denis, J. Desesquelles, M. Druetta, and S. Martin (Université Lyon)
and J.P. Grandin, D. Hennecart, X. Husson, D. Lecler (Université de Caen)
U.V. Spectroscopy of Al IX-Al XII Fine Structure Transitions and Lifetime in Doubly Excited Al XI
12. M. Godefroid (Université Libre de Bruxelles)
A MCHF-BP Study of the J-Dependence of $3s4p\ ^3P_J$ Lifetimes in Mg-like Sulphur and Chlorine

13. Lee E. Howard and Kenneth L. Andrew (Purdue University)
Measurement and Analysis of the Atomic Spectrum of Neutral Arsenic
14. A.S. Bachtijarov and A.A. Nikitin (Leningrad State University),
 P.O. Bogdanovich and Z.B. Rudzikas (Lithuanian Academy of Sciences),
 R. Ch. Salman-Zade (Azerbaijan Academy of Sciences)
On the Structure of the Technetium Spectrum
15. Thomas M. Bieniewski (Los Alamos National Laboratory)
Oscillator Strengths for Neutral Atomic Uranium

Astronomy

C.M. Sitterly, Presiding

Friday, September 16

- 9:00 a.m. George Wallerstein (University of Washington)
Heavy Elements in Cool Stars
- 9:30 a.m. Robert Kurucz (Harvard—Smithsonian Center for Astrophysics)
Millllions and Millllions of Lines
- 10:00-10:25 a.m. Coffee Break
- 10:30 a.m. R.H. Garstang (Joint Institute for Astrophysics, University of Colorado, and National Bureau of Standards)
Hyperfine Structure and the Broadening of Sunspot Spectral Lines
- 11:00 a.m. Bryon A. Palmer (Los Alamos National Laboratory)
Branching Ratios and Lifetimes of Uranium and Thorium Determined from Emission Spectra
- 11:15 a.m. J.K. Crane, G.V. Erbert, J.A. Paisner, S.D. Mostek, L. Prawdzik (Lawrence Livermore National Laboratory)
A New Source for Lifetime Measurements of Refractory Metal Atoms and Their Ions
- 11:30 a.m. N. Grevesse (Université de Liège)
Accurate Atomic Data Needed in Solar Spectroscopy Studies

11:45 a.m.

Earl F. Worden, B. Comaskey, J. Densberger, J. A. Paisner
(Lawrence Livermore National Laboratory),
and John G. Conway (Lawrence Berkeley Laboratory)

*Ionization Potential of Neutral Ion, Fe I, by Laser
Spectroscopy*

12:00 Noon

End of Symposium

RYDBERGS, OPTICAL
RADIATORS, AND
PLANETARY ATOMS

HYPERFINE STRUCTURE AS A PROBE OF STATE MIXING
IN RYDBERG STATES OF ALKALINE-EARTH ATOMS

E. Matthias^{*}

Joint Institute for Laboratory Astrophysics, University of Colorado
and National Bureau of Standards, Boulder, Colorado 80309

In atoms with two valence electrons the magnetic hyperfine structure of $msn\ell$ Rydberg states is determined by three factors¹:

1. the s -electron density at the nucleus;
2. the coupling between the two valence electrons;
3. the influence of nearby states with equal quantum number F .

Accordingly, the hyperfine structure is sensitive to state mixing of various origins.

A change of s -electron density by any admixture of a doubly-excited configuration $n'l'n''\ell''$ into an $msn\ell$ Rydberg series will reveal itself in a change of both the field shift² and, more sensitively, the hyperfine splitting.³ The amount of $n'l'n''\ell''$ admixture can be derived from the data.

The sensitivity of the hyperfine structure to the coupling between the two valence electrons allows us to determine the singlet-triplet mixing caused by configuration interaction. In this case, the amount⁴ as well as the relative sign⁵ of the singlet and triplet mixing amplitudes can be obtained, which, in turn, leads to a significant improvement of the MQDT analysis.⁶

Finally, the hyperfine interaction of the ion core ms electron can mix singlet-triplet,⁷ fine structure,⁸ or neighboring n -states having the same total quantum number F . Such hyperfine-induced state mixing will occur when the states are separated by an energy interval comparable to or less than the hyperfine splitting, and will in general become important or even dominant at very high principal quantum numbers.

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Invited Speaker

OBSERVATION OF QUANTUM DIFFRACTIVE COLLISIONS
USING TWO LEVEL HEAVY OPTICAL RADIATORS

Michael S. Feld

Massachusetts Institute of Technology

Invited Speaker

PLANETARY ATOMS

R. R. Freeman

Bell Laboratories

Angled Beam Photon Echoes R. Beach, B. Brody, M. Glick, P. Yang, and
S. R. Hartmann, Columbia Radiation Laboratory, Columbia University
New York, NY 10027

A photon echo experiment has been performed on the $2^2S_{1/2} - 2^2P_{1/2}$ transition of atomic lithium using non-collinear excitation pulses. The use of non-collinear excitations to generate a photon echo introduces a decay mechanism that provides a measure of the sample's transverse velocity distribution. Our data verifies that the velocity distribution has a Maxwellian form. A notable feature of our experiment is the large dynamic range, nearly 11 orders of magnitude, over which we recorded the decay of echo intensity with increasing pulse separation. Another feature of our data is the absence of echo modulation, as was observed in a similar experiment performed on the $2^2S_{1/2} - 2^2P_{3/2}$ transition in lithium.¹ We also report the results of an experiment done in atomic sodium vapor on the $3^2S_{1/2} - 3^2P_{3/2}$ transition in which we recorded an echo decay over nearly 12 orders of magnitude. In this experiment the smallest echoes observed were from atoms that had lived in their excited state more than 23 natural lifetimes.

The absence of echo modulation as well as the general echo formation process are explained using the Elliptical Billiard Ball Echo model.² This is a refinement of the original Billiard Ball model³ that incorporates the effects of using long, sub-Doller bandwidth excitations in photon echo experiments.

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2. R. Beach, B. Brody, and S. R. Hartmann, Phys. Rev. A 27, 2537 (1983).
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ZEEMAN SPECTRA OF RYDBERG SERIES

W.R.S. Garton, J.P. Connerade, T.A. Stavrakas,
Imperial College, London

J. Hormes, M.A. Baig, B. Alexa
Physikalishes Institut, Bonn

H.M. Crosswhite, H. Crosswhite & F.S. Tomkins
Argonne National Laboratory

We report recent results of collaborative experimental programs at two centers, viz: at Argonne & Bonn.

At Argonne photographic spectra obtained in the second order of the 30 foot Paschen circle, by use of both solenoid and dipole superconducting magnets, have yielded Zeeman spectra of InI in absorption. In addition to the complex structures in high series members associated with diamagnetism and magnetic configuration-mixing, we found the first case reported of simultaneous diamagnetic shift, and partial Paschen-Back Effect. It has been previously supposed that these effects are mutually exclusive. Some quantum-mechanical calculations account semi-quantitatively for the observed structures.

In Bonn we have used the plane-polarized background continuum of the 0.5 gev synchrotron, solenoid magnets and a 3 metre normal incidence spectrograph fitted with a 4900 1/mm holographic grating. For so short an instrument, we achieve high resolution, and believe we report the first resolved Zeeman structures in atomic spectra below 2000 A. In addition the grating has proved to have a strong polarizing property, - in effect acting as an analyser to the plane-polarized light. The result is that each absorption line exhibits a Faraday Rotation pattern superposed on the Zeeman splitting. Measurements of these patterns, and use of classical dispersion theory, provide a means of determination of relative f-values. The method appears to have promising advantages, relative to alternatives of "Hook" or "Equivalent width" techniques, for such determinations in the Schumann U-V.

Rydberg Series $5p^5 6sns$ and $5p^5 6snd$
in the Autoionizing Continua of Neutral Cesium

V. Kaufman, J. Sugar, C.W. Clark, and W.T. Hill, III

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

Abstract

An absorption spectrum of neutral cesium between the $5p^5(2p_{3/2})6s$ and $5p^5(2p_{1/2})6s$ thresholds was observed in the range of 650-700Å with the NBS 10.7-m grazing incidence spectrograph. Rydberg series $5p^5 6sns$ and nd approaching both upper threshold states $(2p_{1/2})6s$, $J=0,1$ were identified on the basis of quantum defect comparisons and Hartree-Fock term energies. Distinctive nd line shapes are compared with those of neutral xenon.

HIGHLY IONIZED

Invited Speaker

SPECTROSCOPY OF HIGHLY IONIZED ATOMS

Brian C. Fawcett

Rutherford Appleton Laboratory

SPECTROSCOPY OF THE NEUTRAL AND SINGLY IONIZED ACTINIDES

Jean Blaise

Laboratoire Aimé Cotton, Campus d'Orsay, 91405 Orsay, France.

The analysis of the actinide spectra began with thorium and uranium during World War II, then Ac I and II, Am I and II, Pu II were investigated and in 1962 the ground states of all the neutral atoms up to curium had been established. The first and second spectra of all the actinides up to einsteinium have now been analyzed, with more success for the even-Z elements than for the others, but most of this work is still unpublished.

The use of even-even isotopes combined with a high resolution instrument (Argonne 9.15 m. Paschen-Runge spectrograph or Fourier transform spectrometer) allows to obtain accurate wavelengths, Zeeman and isotope shift data, while the hyperfine structure of the odd-even isotopes reduces the accuracy of the wavelength measurements and makes it difficult to obtain Zeeman data and, when two odd-even isotopes are available like for Am, isotope shift data. The hyperfine structure itself has been used for the identification of the energy levels: several hundreds of dipole and quadrupole level hyperfine constants could be measured in the Np and Bk spectra while so far, in Pa, Am and Es, only the total splitting of the levels has been determined.

In the absence of configuration mixing one can estimate the isotope shift for various configurations, taking into account the screening of the 7s electron charge density at the nucleus by the 5f, 6d and 7p electrons [1]. The isotope shifts of most of the levels are now known in the spectra of Th, U, Pu, Am and Cm and it has been possible to assign a number of these levels to the proper configuration. Thus far, levels belonging to 13 different configurations of Th I [2] and to 14 configurations of Pu I [3] have been identified, generally confirming Brewer's predictions [4] of the energy of the lowest level of the configurations expected in these spectra from thermodynamic data. If one plots the energy of the lowest level of each identified configuration relatively to $5f^N 7s^2$ or $5f^{N-1} 6d 7s^2$ - both possible ground configurations in the first spectra - one observes a systematic variation which allows to check the assignments of configurations in the spectra for which no isotope shift data are available. Similar plots have been used for the assignments of configurations in the second spectra.

Theoretical interpretations of the configurations following the Slater-Condon theory have been performed but for the complex configurations of elements heavier than Pa, the truncation of the basis set is often necessary. Due to strong overlapping, configuration mixing effects had to be

considered in order to reach a good agreement with the experimental energies and other observables.

In addition to many parametric studies in each actinide element, systematic studies of configurations of the same kind have been made on the whole sequence by the generalized least-squares method, for example $5f^N 7s^2$ and $5f^N 7s$ [5] and $5f^N$ configurations for ions in crystals [6]. Such studies lead to reliable predictions and a substantial progress was made in $5f^{10} 7s^2$ of Cf I and in $5f^{10} 7s$ of Cf II [5].

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Extended analysis of Fe III in the vacuum ultraviolet

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The level structure of doubly ionized iron has been thoroughly investigated by Edlén and Swings [1] in 1942 and by Glad [2] in 1956. In the three lowest configurations, $3d^6$, $3d^54s$ and $3d^54p$, 117 of the 136 possible terms have been established. Many terms in the configurations $3d^54d$, $3d^55s$, $3d^55p$ and $3d^54f$ are also known. Lines in this spectrum appear in many astronomical objects. Therefore there are astrophysical needs for very accurate level energies and also an extension of the term system. It is the aim of the present investigation to provide such results.

The spectrograms used in this investigation were recorded in the 10.7 m normal incidence spectrograph at the National Bureau of Standards, Washington, by using a low-voltage sliding spark discharged. From the spectrograms a wavelength list covering to the region 500 - 2100 Å containing more than 10 000 lines belonging to Fe II to Fe VI have been obtained. All previously observed Fe III lines below 2100 Å are contained in the list and many more can be assigned to Fe III. So far we have determined accurate level values of the previously known levels in the three lowest configurations. Many new lines have been classified as $3d^6 - 3d^54s$ and $3d^54s - 3d^54p$ combinations.

In the present paper we will report on the state of the on going analysis.

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IDENTIFICATION OF THE $ns^0np^6 \ ^1S_0$ LEVEL OF
Ar III AND Kr III BY OPTICAL SPECTROSCOPY

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The $ns^0np^6 \ ^1S$ terms in the spectra of the doubly ionized rare gases were originally identified in Auger-electron spectroscopy. For the heavier rare gases the identifications were based largely on analogy with the identification of the $2s^02p^6 \ ^1S$ term in Ne III. One important difference between neon and the heavier rare gases is that the $n=2$ complex does not contain any d electrons whereas the complexes with $n>2$ involve d electrons. This means that configuration interaction effects are more pronounced for the $ns^0np^6 \ ^1S$ terms with $n>2$ and the analogy between neon on the one hand and argon, krypton and xenon on the other is not quite obvious. As a consequence there has been a lot of discussion about the correct identification of the $ns^0np^6 \ ^1S$ term in the Auger electron spectra of argon, krypton and xenon.

Recently optical emission spectroscopy [1] has been used to verify a proposal by Hertz [2] for the identification of the $5s^05p^6 \ ^1S$ term in Xe III. In particular the optical study showed that the lines involving the $5s^05p^6 \ ^1S$ term were strong in a hollow-cathode discharge but absent in theta-pinch and electrodeless discharges, even though other Xe III lines were of comparable intensity in all three light sources. It was proposed that ion-atom collisions were responsible for the selective population of the $5s^05p^6 \ ^1S$ term in the hollow-cathode discharge. In the present study collision spectroscopy is used to further investigate this mechanism and, at the same time, the mechanism is used to identify the $ns^0np^6 \ ^1S$ terms of Ar III and Kr III.

Using the 600 kV heavy-ion accelerator at Aarhus University we have investigated the cross-section ratios

$$\frac{\sigma(\text{Ne II } 2s2p^6)}{\sigma(\text{Ne II } 2s2p^6)} \quad \text{and}$$

$$\frac{\sigma(\text{Ne III } 2s^02p^6)}{\sigma(\text{Ne III } 2s^02p^6)}$$

and observed that the latter ratio is a factor of ~ 2.5 larger than the former. Since we may expect similar results in studies of He⁺-Ar, Kr systems we have searched for the transitions depopulating the Ar III $3s^03p^6 \ ^1S_0$ and Kr III $4s^04p^6 \ ^1S_0$ levels by comparing the intensities of the spectral lines formed in He⁺-Ar, Kr collisions with the intensities of the identical lines created at the same projectile velocity in Ar⁺, Kr⁺-He collisions.

In parallel, photographic recordings of the spectra of low and intermediate ionization stages of the noble gases, excited in hollow-cathode and theta-pinch discharges, have been used to study the ns^1np^5 - ns^0np^6 transitions in the third spectra of the rare gases. The spectrograms, recorded on the 3-m normal-incidence vacuum spectrograph at Lund Institute of Technology, facilitate an accurate determination of the position of the 1S term, the uncertainties in the level values being of the order of 0.0001 eV. As has previously been observed for xenon the ns^0np^6 1S term of neon, argon and krypton is strongly populated in a glow-discharge as compared to a theta-pinch discharge.

The present results verify the assignments by McGuire [3] in the Auger-electron spectra of argon and krypton. A comparison between the experimentally determined relative positions of the ns^2np^4 , ns^1np^5 and ns^0np^6 configurations and theoretical predictions based on Hartree-Fock calculations reveals that the correlation energies are at a maximum for argon and then decreases regularly with increasing nuclear charge.

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The $4d^9 5s 5p$ configuration in I VII through Eu XVII

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ABSTRACT

The spectra were produced with a high voltage spark discharge and photographed with the N.B.S. 10.7m grazing incidence spectrograph. The Ag I-like transition array $4d^{10} 5s - 4d^9 5s 5p$ was first identified by comparison with the analogous array in the Cu I isoelectronic sequence, then by comparison with a calculated spectrum. The latter was obtained with scaled Hartree-Fock radial energy integrals. The transition array $4d^{10} 5s - 4d^9 5s 5p$ has been observed most completely in I VII and Xe VIII, and with decreasing strength to higher sequence members. In Sm XVI and Eu XVII only the strongest line was found. Results of the calculations for I VII and Xe VIII will be given.

A tracing of the array for Xe VIII is given in fig. 1 where the peaks are labeled to correspond with those of the Cu I sequence. The two strong lines of the Pd I sequence³ ($4d^{10} - 4d^9 5p$) are at 165.327 Å and 161.738 Å, just to the short wavelength side of the array in fig. 1. On the long wavelength side are the two lines of $4d^{10} 5s^2 - 4d^9 5s^2 5p$ of Xe VII, denoted by triangles. Fig. 2 shows the Cu I-like array of $3d^{10} 4s - 3d^9 4s 4p$ of Zr XII with the two Zn-like lines $3d^{10} 4s^2 - 3d^9 4s^2 4p$ of Zr XI from ref. 1.

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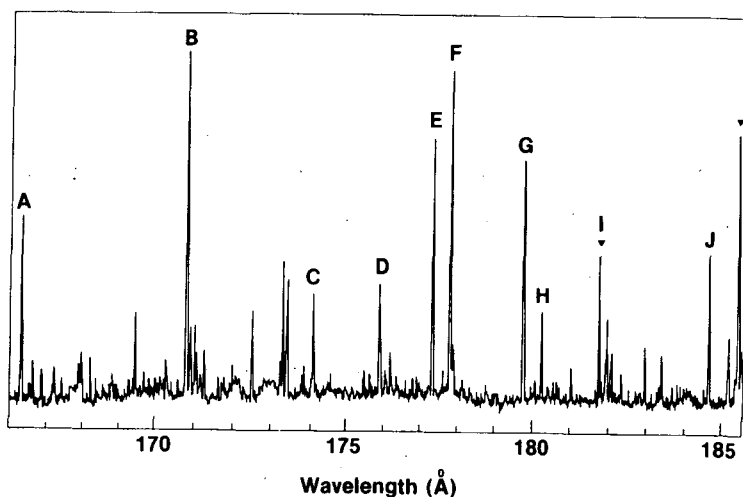


Fig. 1. The $4d^{10}5s-4d^9 5s5p$ transition array of Xe VIII in which alphabetic labels identify members of the array as in fig. 2. Triangles denote lines of $4d^{10}5s^2-4d^9 5s^2 5p$.

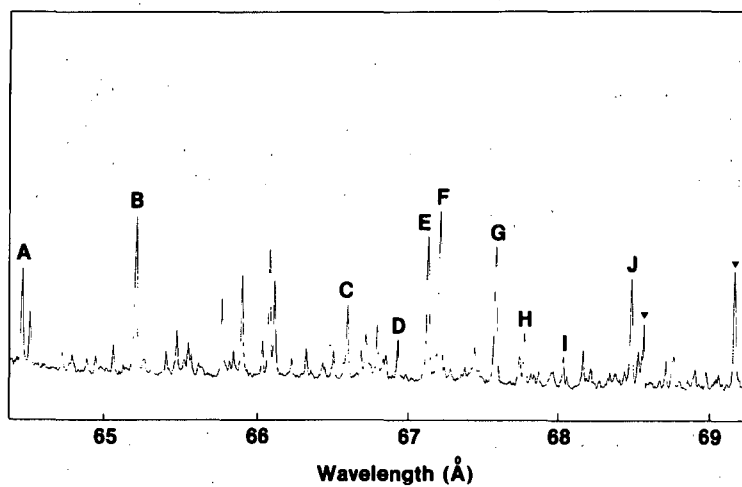


Fig. 2. The $3d^{10}4s-3d^9 4s4p$ transition array of Zr XII labeled as in ref. 1. Triangles denote lines of $3d^{10}4s^2-3d^9 4s^2 4p$.

The Atomic Spectrum of Neutral Gold

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The emission spectra of a gold hollow cathode lamp was recorded with the Kitt Peak National Observatory Fourier transform spectrometer from about 270 nm in the ultraviolet to beyond 2 μm in the near infrared. Previously assigned lines of Au I and a few new transitions were accurately measured. A least squares refinement of these assigned lines yielded a set of Au I levels accurate to a few thousandths of a cm^{-1} . This is somewhat more accurate than the level list given by Ehrhardt and Davis [JOSA, 61, 1342(1971)], but our analysis is in agreement with theirs. The allowed ground state lines of Au I lie beyond the ultraviolet cutoff of our spectra. However, the measurement of the forbidden ground state line at 21434 cm^{-1} allowed us to accurately determine the ground state interval. Some hyperfine patterns were observed and analyzed. A few lines of Au II were also measured accurately.

THE SPECTRUM OF DOUBLY IONIZED TUNGSTEN, W III

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The spectrum of tungsten was photographed between 600 and 2660 Å on the 10.7-m spectrograph at the NBS using as light source a sliding spark under different excitation conditions. About three thousand lines have been attributed to the W^{++} ion (W III) and this paper presents the first analysis of the spectrum.

The low even configurations are: $5d^4$ and $5d^3 6s$. More than half of the predicted levels of these configurations have already been found, in agreement with the calculated values.

Near one hundred levels belonging to the odd configurations $5d^3 6p$ + $5d^2 6s6p$ have also been determined. Theoretical calculations, including configuration interaction, have been done. The assignment of levels to the corresponding electronic configuration is rather difficult especially for some of the high $5d^3 6p$ and the low $5d^2 6s6p$ levels.

The analysis is in progress.

ULTRAVIOLET

Atomic Inner-Shell Transitions*

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In several important aspects, atomic inner-shell processes have quite different characteristics from those in the optical regime. Energies are large, with the 1s binding energy reaching 100 keV at $Z \approx 87$; relativistic and quantum-electrodynamic effects are strong. Isolated inner-shell vacancies have pronounced single-particle character, with correlations generally contributing less than 1 eV of the energy of [1s] and [2p] hole states; the structure of such systems is thus well-tractable by independent-particle (SCF) atomic models. Hole-state lifetimes are short, of the order of attoseconds to femtoseconds; there are many decay channels and some transition rates are exceedingly strong. Time-dependent perturbation theory is thus driven to its limits, and the traditional separation of atomic excitation from the deexcitation phase breaks down, especially near threshold. Studies of inner-shell processes through synchrotron-radiation and ion-atom collision experiments can consequently provide access to interesting, little-explored phenomena.

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Invited Speaker

SPECTROSCOPY OF X-RAY LASERS

R. C. Elton

Naval Research Laboratory

LASER SPECTROSCOPY IN THE EXTREME ULTRAVIOLET

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The paper will describe several new techniques for using lasers for high resolution spectroscopy of core-excited atomic levels. The techniques discussed will include: anti-Stokes absorption spectroscopy, anti-Stokes emission spectroscopy, and a new technique which may be termed as extinction spectroscopy. Methods of producing large densities of alkali quartet atoms will also be described.

Subnatural Linewidth Effects in Polarization Spectroscopy

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Recently we have reported on a new method for the production of optical resonances which are narrower than the natural width of a spectral line [1]. The method has first been applied to Na and is based on the technique of polarization spectroscopy [2,3]. The principal difference, however, is that the linearly polarized probe beam perturbs the investigated medium about as strongly as the circularly polarized pump beam. The main feature observed in these experiments is an additional dip in the standard Doppler-free polarization spectroscopy signal, whose depth, width and position depend on the intensities of the light beams, on the angle between polarizer and analyzer and on the pressure in the resonance cell. Dips with a linewidth as narrow as 2.6 MHz (see Fig.1), i.e. considerably narrower than the natural width of 10 MHz have been observed [1].

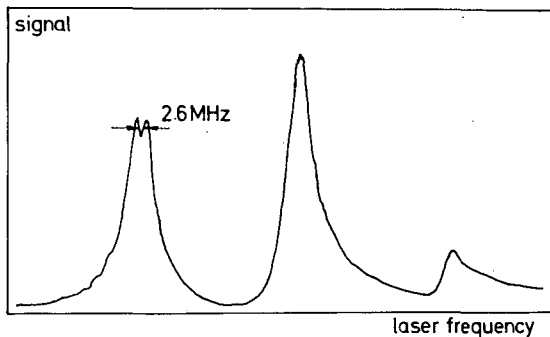


Fig.1 An example of the narrowest dips in the Na-D1-line with a linewidth of 2.6 MHz.

In the present paper we report on a new series of experiments which have been started to elucidate further the mechanisms that are responsible for the new signals with subnatural linewidth. The main goal was to distinguish between two interpretations of the signals. Firstly, the resonances might be due to Zeeman coherences induced by the two laser beams and revealed in the signal by velocity selective light shifts while scanning the laser frequency [1]. On the other hand, in the case of sodium, Zeeman or optical hyperfine pumping can also be responsible for the observed effects. In particular, subtle nonstationary effects of velocity selective optical pumping have recently been shown to result in similar lineshapes of Doppler-free two-photon resonances in Na [4].

So far, the following tests have been performed:

- i) The interaction time of the atoms with the laser light fields has been varied by changing the diameter of the beams. This strongly influences the shape of the signals (see Figure 2a,b)
- ii) Measurements have been performed on the Na $^2S_{1/2}$ F=2 - $^2P_{3/2}$ F=3 transition, where neither hyperfine nor Zeeman pumping can take place. Here no dip could be observed.
- iii) As a possibility for the direct detection of light shifts of different Zeeman levels an rf-field was applied to induce magnetic dipole

transitions. The rf-frequency was varied from several kHz to 10 MHz. The only effect was a decrease of the signal as a whole, i.e. the direct test on the model with Zeeman coherences and light shifts was negative.

In addition to the experiments outlined above, theoretical calculations have been performed using a four level system that accounts for Zeeman as well as hyperfine optical pumping. After analytical solution of time dependent rate equations and numerical integration over the transversal and longitudinal velocity distributions theoretical signals have been obtained. They are in close agreement with experiment and, in particular, reproduce dips with subnatural linewidth and with the properties mentioned above. Thus, the experimental tests as well as the calculations support the idea that the narrow structures in typical polarization spectroscopy signals are due to nonstationary effects of optical pumping.

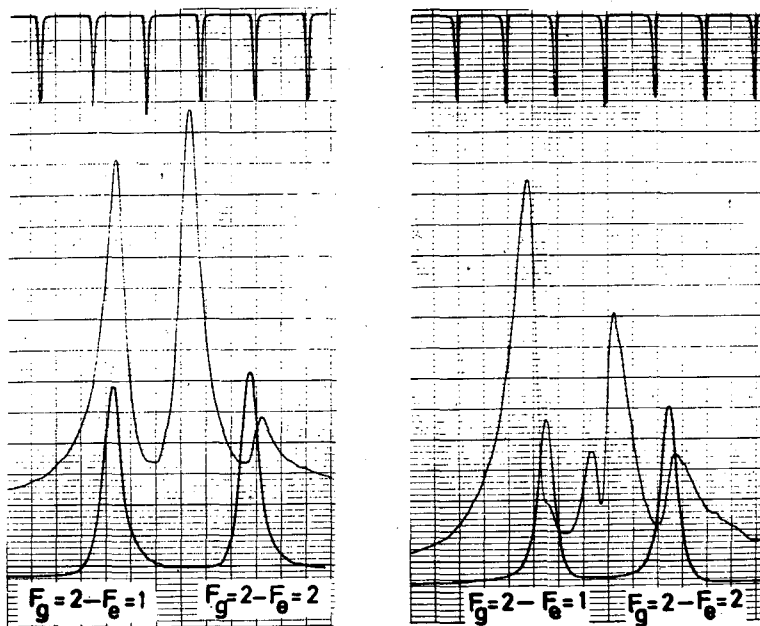


Fig.2 Polarization spectroscopy signals (upper traces) obtained with a strong probe beam of different diameter ϕ a) $\phi = 0.5$ mm and b) $\phi = 7.5$ mm where additional structures in the signals become visible. The pump beam diameter was $\phi = 8$ mm. The lower traces represent resonance fluorescence signals recorded simultaneously with a collimated atomic beam for reference purposes.

In conclusion, we want to emphasize the importance of optical pumping effects in polarization spectroscopy. A thorough analysis of these features is necessary for a correct understanding of the recorded lineshapes and consequently for the achievement of high precision. We have demonstrated how dips can be produced that are located at the center of the optical transition and may be significantly narrower than its natural width. However, it should be noted that the new dips are not Lorentzian and in spite of their subnatural width it is not possible to exceed the resolution limits imposed by the natural linewidth.

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Method for Signal Enhancement in Laser Spectroscopy of Metastable States

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Doppler-free laser spectroscopy on weak transitions associated with narrow resonances permits measurements of the highest resolution and precision suitable even for time and length standards [1]. However under most experimental conditions only a very limited number of photon absorption/emission processes per atom is possible during the interaction with the laser light. Hence the signal-to-noise ratio can be rather poor. This is particularly disadvantageous in applications such as laser stabilization where the center frequency of a resonance has to be determined continuously with a short time constant so that signal averaging techniques cannot be applied.

We have therefore performed experiments with the goal of combining high resolution with high sensitivity in laser spectroscopy. The idea underlying our studies is to transfer a narrow signal with a second cw laser from a weak transition to a strong resonance line. The experiments reported here were stimulated by Ramsey fringe spectroscopy in a calcium atomic beam. Several groups have carried out such experiments [1,2] on the very weak Ca-intercombination transition connecting the $4s^2\ ^1S_0$ ground state with the metastable ($\tau = 0.4$ ms) $4s4p\ ^3P_1$ excited state (see Fig.1). This line with a natural width of only 410 Hz is suggested as an optical frequency standard with a reproducibility of 10^{-14} [3]. Although ultra-narrow Ramsey resonances have already been observed, applications as a standard are presently hampered by integration times of several minutes. Therefore, improvements of the signal-to-noise ratio are highly desirable and have recently found additional motivation by the demonstration of longitudinal Ramsey fringe spectroscopy [3] where earlier limitations due to second-order Doppler broadening can be overcome.

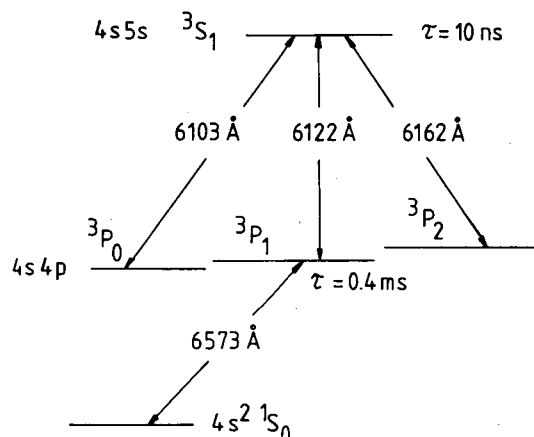


Fig.1: Part of the energy level diagram of calcium

Our experimental arrangement is shown schematically in Fig.2. The atoms first travel across the beam of a single-mode cw dye ring laser with $\lambda = 6573\ \text{\AA}$ which produces a narrow Doppler-free signal in the intercombination transition. Due to the long lifetime of the 3P_1 state the reemitted resonance fluorescence light can be registered some 50 cm downstream of the atomic beam [4]. A few centimeters behind the first laser beam the atoms pass a second laser light field with $\lambda = 6122\ \text{\AA}$. Here, excitation from the $4s4p\ ^3P_1$ state to

the short-lived $4s5s\ ^3S_1$ level ($\tau=10$ ns) is accomplished. To make the scheme as simple as possible a laser in broadband operation was used for this second step. A fast modulation of the cavity length assured that a quasi-continuous spectrum was emitted. Since the atoms interact consecutively with the two light fields, the Doppler-free signals can be transferred without additional broadening from the intercombination line to the $^3S_1 - ^3P_{0,1,2}$ transition.

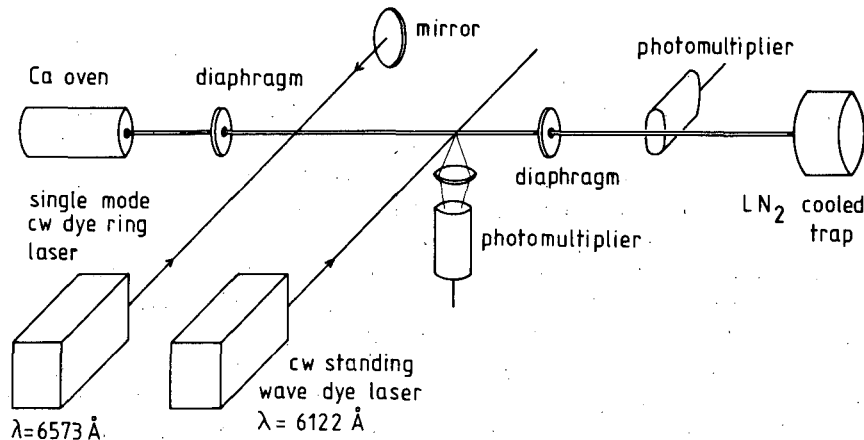


Fig.2: Experimental arrangement for signal enhancement of Doppler-free signals in the Ca intercombination transition.

Although the application of one additional laser for the line $^3P_1 - ^3S_1$ does not markedly increase the number of photons emitted per atom because of the partial decay into the 3P_0 and 3P_2 -states, the signal-to-noise ratio can be increased by a factor as large as 25. This is possible because the prompt fluorescence from the 3S_1 state is emitted from a rather small resonance volume, whereas the decay of the longlived 3P_1 level takes place along the path of flight of the atomic beam with a decay length of 20 cm. Therefore, photons emerging from the decay of the 3S_1 state can be collected and detected easily which is not possible for the 3P_1 level. The first experiments yielded an enhancement of the signal-to-noise ratio of about a factor 5-10. At the same time the fluorescence signal of the intercombination line decreases to one third of its original value due to optical pumping into the 3P_0 and 3P_2 states. The detection scheme via the $^3P_1 - ^3S_1 - ^3P_2$ levels offers the additional advantage of complete optical isolation of the exciting and detected wavelengths. Presently further studies including non-optical detection schemes are under way.

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Ultraviolet Laser Spectroscopy of Doubly Charged Europium Ions

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The Eu^{2+} ion is of particular interest since its spectroscopic properties are of relevance to important problems in physics and astronomy. For example, transition probabilities of spectral lines (see Fig.1), that can be derived from lifetime measurements, are needed for the calculation of the europium abundance in peculiar stars such as the magnetic Ap stars [1]. Here, Eu seems to be orders of magnitude more abundant than in the solar system. Another example illustrating the importance of spectroscopic measurements on free Eu^{2+} ions is the variation of the ground state hyperfine structure (hfs) splittings of Eu^{2+} in crystals of different type and chemical composition [2]. A precise measurement of these splittings for the free ion would permit to study quantitatively how the magnetic dipole and the electric quadrupole interactions of the imbedded Eu^{2+} ion are modified by the surrounding ligands. Also, the influence of a covalent contribution to the bonding in ionic crystals and possibly of zero-point lattice vibrations on the magnetic hfs can be evaluated [3]. So far, this important information is not available since, to the authors' knowledge, no hfs measurements exist for any free ion as well as the same ion implanted in a crystal.

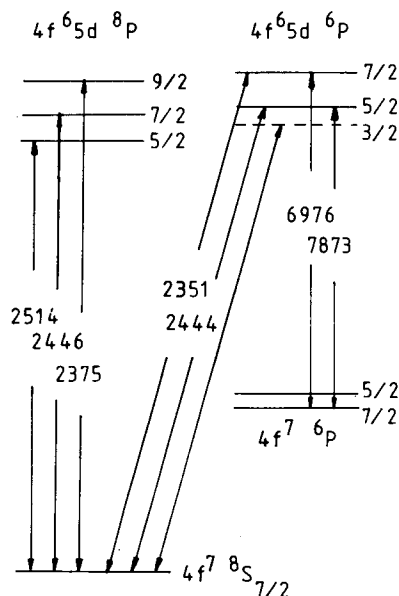


Fig.1 Part of the energy level diagram of Eu^{2+} . All wavelengths are given in Ångstroms.

We have attacked the questions outlined above and first developed a source for thermal Eu^{2+} ions. Europium atomic vapour is produced in a resonance vessel by heating the metal in a temperature stabilized oven. Ions are created by driving a steady gas discharge above the orifice of the oven (see also ref.[4]). The discharge current is carried by an inert buffer gas at a pressure of several Torr. A coaxial arrangement with annular electrodes was chosen in order to avoid magnetic fields due to the discharge current. The vacuum system of the apparatus is equipped with components for circulation and purification of the buffer gas. After careful optimization of all parameters,

Eu^{2+} ions of considerable density ($n \approx 10^8 \text{cm}^{-3}$) could be produced. Eu^{2+} was identified by recording the emission spectrum of the discharge (see Fig.2) where most of the Eu^{2+} lines, shown in Fig.1, could be observed unambiguously and with good signal-to-noise ratio.

As a second step of this experiment lifetime measurements of the $4f^6 5d^6 p$ and $8p$ excited states of Eu^{2+} have been started. A nitrogen laser pumped dye laser system with a pulse duration of about 2 ns is used for this purpose. The output is frequency doubled in a nonlinear KPB crystal in order to generate UV light necessary for the excitation of the Eu^{2+} ions. The reemitted resonance fluorescence light is detected by a fast photomultiplier. With a sampling oscilloscope time resolved signals are registered. They are stored in a multichannel analyzer (see Fig.2). First results indicate that the lifetimes are of the order of a few nanoseconds.

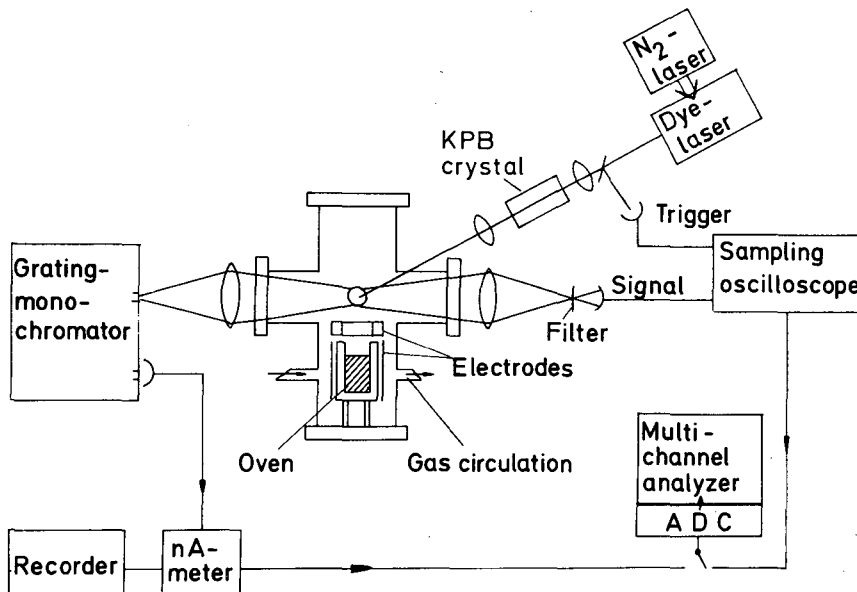


Fig.2 Experimental arrangement for lifetime measurements of Eu^{2+} ions.

Presently, experiments are being started in order to investigate two-photon transitions in free Eu^{2+} . Additionally, measurements of the ground state hfs are in preparation. This requires the generation of narrow-band continuous wave UV laser light with $\lambda \approx 2500 \text{ \AA}$ by sum frequency mixing of a monomode dye laser in the far red and a UV single-frequency Ar^+ laser. It is planned to apply the technique of combined optical-pumping microwave spectroscopy in order to obtain the Eu^{2+} ground state hfs splittings with a precision of 10^{-5} .

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POSTERS

NOTES

First and Second Spectra of Transition and Light Metals
in the 1-5.5 Micron Region by Fourier Spectroscopy

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Using a simple water cooled hollow cathode with demountable cathodes, rich spectra of a number of transition and light metals have been obtained in the 1-5.5 micron region with the Fourier transform spectrometer at the McMath telescope of Kitt Peak National Observatory. Helium, neon, and argon, as well as mixtures of pairs of these gases, have been used as carriers in the flow-through system, thus providing different degrees of excitation. Observations were made at a resolution of 0.01 cm^{-1} , and the dynamic range in the spectra is commonly 10^4 or 10^5 to 1. Atlases of portions of these spectra, including samples of Iron, Nickel, Titanium, Vanadium, Copper and Magnesium spectra, will be available for inspection.

ATOMIC LEVEL POPULATIONS IN THE HOLLOW CATHODE SPECTRAL LIGHT SOURCE

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The relative populations of 76 Fe I levels have been measured in a Fe + Ar hollow cathode discharge operating under conditions (1.5 Torr, ≤ 100 watts in a cathode of 3 mm I. D. by 18 mm long) typical for a thin spectral source. Emission line intensities were recorded with the 1-meter Fourier transform spectrometer⁽¹⁾ at the Kitt Peak National Observatory, and the level population was derived from the line intensity with the precise gf-values of Blackwell et al⁽²⁾. For many levels the population was derived from several decay branches and the independent values were averaged.

The populations do not follow a Boltzmann distribution: levels at nearly the same excitation energy may differ in population by a factor of ten. The population of a level is found to increase with the radiative lifetime τ of the level until τ exceeds the mean time T_Q between quenching collisions. The radiative lifetimes used in this analysis were taken from the literature or computed from the Blackwell et al gf-values and emission branching ratios measured in this experiment.

The gross features of the population distribution suggest a mechanism whereby all excited levels are populated at an equal rate, independent of excitation energy, so that the equilibrium population is proportional to an effective lifetime $T = (\tau^{-1} + T_Q^{-1})^{-1}$ with $T_Q \approx 10^2$ ns for all levels. This crude model does not account for a distinctive feature of the population distribution reported earlier by Crosswhite⁽³⁾: for levels within the same term of nearly the same radiative lifetime, the population decreases smoothly with increasing excitation energy, as if mixing collisions established a statistical equilibrium for levels within a term.

The carrier gas is not critical: Ne and Ar lead to Fe I level population distributions that are indistinguishable. The molybdenum level distribution in a Mo + Ar source displays the same dependence on the effective lifetime of the level observed with iron. A few Ar I and II and Fe II level populations have been measured but with less accurate gf-values and too few to show the features observed with Fe I and Mo I.

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* Guest observer, Kitt Peak National Observatory, operated by AURA under contract with the NSF.

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Laser-Produced Spectra of Copperlike Ions from Ru¹⁵⁺ to Sn²¹⁺

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As part of a continuing study¹⁻⁹ of the copper isoelectronic sequence, we have now obtained spectra of the ions Ru¹⁵⁺, Rh¹⁶⁺, Pd¹⁷⁺, Ag¹⁸⁺, Cd¹⁹⁺, In²⁰⁺, and Sn²¹⁺ with a laser-produced plasma at NBS. Typical laser pulses had an energy of 15 J and a duration of 15 ns. The spectra were observed with a 10.7-m grazing incidence spectrograph. The region of observation was 39-374Å. Wavelengths, energy levels, and ionization energies were obtained for each ion. By means of the Ritz combination principle, accurate wavelengths could be determined for several n=4-5 transitions in the 45-68Å region. The results are compared with the relativistic Hartree-Fock calculations of Cheng and Kim.¹⁰

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Accurate Wavenumber Measurements for the ^4He I $1s2p-1s3d$ Transitions

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We have measured the ^4He $2\ ^3P-3\ ^3D$ (5875 Å) and $2\ ^1P-3\ ^1D$ (6678 Å) lines observed by Doppler-free intermodulated fluorescence spectroscopy, and also the spin-forbidden $2\ ^1P_1-3\ ^3D_2$ (6679 Å) and $2\ ^3P_{1,2}-3\ ^1D_2$ (5874 Å) lines observed in Doppler-limited fluorescence spectra. The wavenumber of the tunable dye laser inducing the fluorescence was measured relative to an iodine-stabilized He-Ne laser by the classical method of photographic Fabry-Perot interferometry. The uncertainties of the Doppler-free measurements and of the $2\ ^1P_1-3\ ^3D_2$ determination are 10^{-4} cm^{-1} or less (3 MHz). Our $2\ ^3P-3\ ^3D$ results agree with the recent measurement by Hlousek et al. [1] and are in marginal disagreement with the measurements by Juncar et al. [2].

Our value for the intersystem $2\ ^3P-2\ ^1P$ separation, together with existing calculations, indicates that the Lamb shift of $2\ ^1P$ is less than 0.01 cm^{-1} (absolute value), this result also being indicated by comparison of our $2\ ^1P-3\ ^1D$ measurement with theory. Combination of the $2\ ^3P-3\ ^3D$ measurements with an experimental value for the $2\ ^3S-3\ ^3D$ separation [3] gives a value for the $2\ ^3S-2\ ^3P$ separation that can be compared with available calculations to obtain an experimental value of the $2\ ^3S-2\ ^3P$ Lamb shift. The result is $-0.1776(5)\text{ cm}^{-1}$, as compared with a calculated value of -0.173 cm^{-1} [4]. The new value for the $3\ ^3D-3\ ^1D$ separation has been used with a known value for this separation in ^3He [5] to obtain experimental values of $-243(18)$ and $-322(24)$ MHz for the mass-polarization contributions to this singlet-triplet separation in ^4He and ^3He , respectively [6]. Combination of our measurements with the accurately known $2\ ^3P_0-^3P_1$ interval gives a value of $1325.4(2.0)$ MHz for the $3\ ^3D_1-^3D_2$ interval, consistent with several previous determinations. In addition to the mass-polarization energy, we have derived new parametric values for the other ^4He $1s3d$ interactions (three magnetic interactions and the exchange energy) and for the singlet-triplet mixing coefficient.

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Compilations of Atomic Energy Levels*

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Abstract

We have been publishing new compilations of energy levels for single elements in all stages of ionization as each is completed. Those now in print in the Journal of Physical and Chemical Reference Data are helium (1973), sodium (1981), magnesium (1980), aluminum (1979), silicon (1983), potassium (1979), calcium (1979), scandium (1980), titanium (1979), vanadium (1978), chromium (1977), manganese (1977), iron (1982), cobalt (1981), and nickel (1981). A volume containing atomic energy levels of all the rare earth elements was issued in 1978. We are now bringing up-to-date our compilations in the iron period (K through Ni, 235 spectra), which will be published in a single volume.

We also publish bibliographies of works dealing with atomic energy level and wavelength data. The last bibliography appeared in 1980 and covered the period 1975 to 1979. Our next issue will extend through Dec. 1983. Work continues on the table of wavelengths for atoms in the first five ionization stages, published as NSRDS-NBS 68, with updated tables given annually in the Handbook of Chemistry and Physics.

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CRITICAL COMPILATIONS OF ATOMIC TRANSITION PROBABILITIES*

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The staff of the NBS Data Center on Atomic Transition Probabilities is currently engaged in the critical evaluation and compilation of atomic transition probabilities for both allowed and forbidden transitions of the iron-group elements scandium through nickel in all stages of ionization. This compilation constitutes a revision, expansion and updating of a series of smaller NBS compilations which appeared in the Journal of Physical and Chemical Reference Data over the last several years.

The world literature on atomic transition probabilities is searched, collected, and catalogued on an ongoing basis by the Data Center. A master reference list is maintained, and annotated bibliographies are issued from time to time as the number of new articles in the literature and the resources of the Center permit.

Exchange of information between the Center staff and both producers and users of transition-probability data is encouraged. In addition to the published compilations and bibliographies, user services include responding to requests, through the mail or by telephone, for data and for new references (i.e., those which have not yet been included in a published bibliography), as well as reception of visitors to the Center for use of the files and consultation on technical matters. Receipt, from professionals in the field, of research results in advance of publication is welcomed, so that the Center staff can incorporate these data into the critical evaluation/compilation process to the greatest extent possible.

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Wavelength Measurements of 2s-2p Transitions in
Flourinelike and Oxygenlike Krypton XXVIII and XXIX*

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We have measured wavelengths of the 2s-2p doublet in flourinelike Kr XXVIII and several 2s-2p transitions in oxygenlike Kr XXIX. The spectra were produced using a linear hollow gas puff z-pinch driven by the PITHON relativistic electron beam generator at Physics International. The resulting Z-pinch plasma was viewed radially with radial spatial resolution. The spectra were recorded in 101-05 film using a 1-meter grazing incidence spectrograph at an angle of incidence of 2° and fitted with a 1200 gr/mm. grating. The absolute uncertainty in the wavelengths is estimated at ±.03Å while the uncertainty in the relative spacings is felt to be ±.013Å.

Table I contains our current results. Identifications are based on interpolations/extrapolations along isoelectronic sequences, comparisons with ab initio calculations¹ and correlations of the spatial extent of the emitting regions with the plasma parameters. For the transitions belonging to the oxygen isoelectronic sequence we used an extrapolation technique due to Edlen² where we fit a polynomial of low order to differences between observed values and ab-initio calculations.

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¹J. Scofield, private communications.

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Table I. Wavelengths of Krypton Lines

<u>ION</u>	<u>CONFIGURATION</u>	<u>L-S</u>	<u>J-J</u>	<u>LAMDA</u>
KrXXVI	4f-5g	² F- ² G	5/2-7/2 7/2-9/2	59.45
KrXXVIII	2s ² 2p ⁵ -2s2p ⁶	² p- ² S	3/2-1/2 1/2-1/2	52.60 68.75
KrXXIX	2s ² p ⁴ -2s2p ⁶	³ p- ³ P	2-1 1-0 0-1 2-2	53.64 58.49 58.69 59.71
		¹ D- ¹ P	2-1	53.97

New Technique for X-ray Line Measurements in
Fast Ion Spectroscopy*

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A Johann type curved crystal spectrometer has been constructed for use in fast ion beam foil spectroscopy. The spectrometer uses a coplanar crystal pair in a geometry that provides a direct determination of the linear doppler shift and a measurement of the beam velocity. The geometry removes the constraint of narrow angular acceptance found in flat crystal spectrometers resulting in more than an order of magnitude improvement in sensitivity without any loss in spectral resolution. The spectrometer provides simultaneous measurements over a wide range of Bragg angles $\sim 30^\circ$ - 70° . The theory of the spectrometer as well as important design and performance parameters will be discussed.

The spectrometer has been installed at the Lawrence Berkeley Laboratory Heavy Ion Linear Accelerator. The high efficiency of the spectrometer allowed useful data to be obtained in only 20 minutes at a beam current of 1 microamp at a resolving power of 2500. Preliminary results using Fe beams will be presented. In particular, the measurement of the $2P_{3/2} - 2P_{1/2}$ fine structure splitting in hydrogenic iron will be presented. The measured fine structure separation is in better agreement with theory than the previously reported value of Briand¹.

*Work performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under contract number W-7405-ENG-48.

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Rydberg levels of alkaline-earth spectra : MQDT wavefunctions probed
by laser measurements

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The high-Rydberg states of heavy alkaline earth-atoms, Ca, Sr and Ba have received considerable attention during the last decade. Here is shown how the interplay of laser experiments and theoretical analyses with MQDT (Multichannel Quantum Defect Theory) has permitted to greatly extend the understanding of the detailed structure of these two-electron systems.

The major motive for the interest in the alkaline-earth spectra is the ability to study interacting Rydberg series. The perturbations of principal Rydberg series $m_0s n\ell$ by doubly excited states $(m_0-1)d n'\ell'$ and m_0p^2 are reflected not only on the level structure but also on various observable quantities - oscillator strengths, lifetimes, g_J Landé factors, hyperfine structures, isotope shifts, In the same way, above the first ionization limit, not only the position of autoionized levels, but also the shape and width of their profiles largely depend on channel mixing.

From a theoretical point of view, MQDT is a powerful tool for studying interacting Rydberg series. In Ca, Sr and Ba successful parametrizations of the observed spectra were carried out. However a crucial point, emphasized here, is that energy values often represent a too limited data set to get the full MQDT parameters needed to determine the wavefunctions. Relative signs of mixing coefficients can never be inferred from energies and MQDT parametrizations of energy levels are based on some hypotheses. Data on observable quantities other than energies are required to remove the partial indeterminacy of MQDT parameters and to probe the validity of the assumptions.

Laser experiments, mainly high-resolution spectroscopy, have provided recently the possibility of analyzing state mixing and intermediate coupling of high Rydberg states. Here is shown how the informations provided by different measurements complement each other to check and even extend MQDT models derived from energies. This point is illustrated by various examples mainly concerning the even-parity spectrum of Ba which was the most extensively investigated. In this complex spectrum governed by the mutual influence of electrostatic interaction and spin-orbit coupling, g_J factor and hyperfine structure measurements are essential to improve MQDT wavefunctions.

The Third Spectra of Uranium and Thorium

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Hollow cathode lamp spectra of uranium and thorium covering the region from 250 nm to 5 μ m have been examined for doubly ionized spectral lines. The spectra were obtained on the Kitt Peak National Observatory Fourier transform spectrometer. In the thorium spectrum, we have improved the energy level values by two orders of magnitude and have located and identified new transitions. The thorium spectrum has previously been analyzed with better excitation sources for the third spectrum so no new levels were located. The doubly ionized spectrum of uranium has not been analyzed. Therefore only those lines which previously were identified as potential third spectrum lines and those lines we have identified are presented. The energy level structure of U III will be discussed.

Detailed Analysis of 4-2, 3-2 and 3-3 Emission Spectra from
Neon-like and Near Neon-like Krypton Produced in a Z-Pinch Plasma*

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Interest in neon-like systems produced in high density plasmas has increased because these ions have potential application as a medium which can produce stimulated UV or soft x-ray emission. The spectroscopic analysis of neon-like systems is difficult because relatively little work in this area, particularly for 3-3 transitions, is available. Firm identifications of 3-3 transitions for neon-like argon has been reported from beam-foil measurements¹ and tentative identifications for iron are available². Analysis of data is very difficult because there are a large number of 3-3 transitions involving ions near the neon-like sequence. Clearly more work in this area is required. The use of high density z-pinch provides an excellent tool for doing this work. The high density and temperatures attainable in z-pinch allow the observations for highly stripped systems of both resonance and multiply excited systems.

In this paper we report spectroscopic measurements of 4-2, 3-2 and 3-3 transitions (where the numbers refer to the principal quantum number) of neon-like and near neon-like ions obtained in a krypton plasma. The plasma was produced in a gas puff z-pinch obtained at the Python generator at Physics International. The spectral lines were observed with two crystal and two grazing incidence spectrometers. All spectrometers provided spatial resolution and for the grazing incidence spectrometers the plasma was observed both axially and radially. The wavelength calibration for the grazing incidence spectrometer was obtained from pinches involving argon and krypton mixtures and using the well known 2-2 lines of argon. The positions of the argon lines was compared with calibration lines of aluminum and oxygen obtained from a capillary discharge. The experimental uncertainties in the measured positions of the line centers for 3-3 krypton transitions in the 100 to 250 Å region is .03 Å.

In the grazing incidence spectra approximately 100 lines between 100 and 250 angstroms have been detected. A small fraction of these lines have been identified using the semi-empirical extrapolation technique of Edlen³. These lines correspond to resonance 3-3 transitions in 11, 12, and 13 electron systems. The majority of the remaining lines have been tentatively identified as doubly excited 3-3 transitions in 11, 12, and 13 electron systems and 3-3 transitions in a variety of neon-like configurations. The tentative identifications are based on empirical

corrections to relativistic Hartree-Fock calculations and detailed atomic modeling of the expected line intensities. Copious lines are observed in other regions of the grazing incidence spectra and these lines will be discussed.

Several x-ray spectral measurements obtained using mica, PET and KAP crystals have been analyzed. Identifications of the lines are consistent with 4-2 and 3-2 transitions in 8, 9, 10, 11 and 12 electron systems. In some spectra simultaneous observations of transitions involving 1 and 2 electron argon and phosphorous are observed. The mean plasma temperature and density have been obtained from the impurity data. Comparisons between our data and theoretical predictions of ionization balance for the krypton plasma, using the measured plasma parameters will be presented.

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THEORY

NOTES

Theoretical Procedures for Atomic Energy Levels

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One of the most disconcerting features of fitting atomic energy levels to parameters is that the addition of a new parameter usually entails significant changes to the old ones. For example, the term energies $E(^{2S+1}L)$ for d^2 are given in terms of the Slater parameters F_k by

$$\begin{aligned} E(^1S) &= F_0 + 14F_2 + 126F_4, & E(^3P) &= F_0 + 7F_2 - 84F_4, \\ E(^1D) &= F_0 - 3F_2 + 36F_4, & E(^3F) &= F_0 - 8F_2 - 9F_4, \\ E(^1G) &= F_0 + 4F_2 + F_4. \end{aligned} \quad (1)$$

If an improved fit to the experimental term energies is sought by adding the Trees correction $\alpha L(L+1)$ to the right-hand sides of these equations, then the fitted values of the F_k can be expected to change. In a similar way, the inclusion of the additional corrections $5\beta\delta(v, 0)$ of Racah, where v is the seniority, will in general produce further changes to the F_k and also to α . For configurations more complex than d^2 we may want to hold open the possibility of adding a succession of corrections. It would be highly convenient if these corrections could be put in a form that produced insignificant changes to the parameters already determined. For energies E that depend linearly on the parameters p_i , this can be achieved by picking associated operators H_i , assumed scalar with respect to rotations in ordinary three-dimensional space, for which

$$\sum (2S_\psi + 1)(2L_\psi + 1) \langle \psi | H_i | \psi' \rangle \langle \psi' | H_j | \psi \rangle = 0, \quad (i \neq j) \quad (2)$$

the sum running over the terms ψ and ψ' (with common S_ψ and L_ψ) of a configuration.¹ Contingent requirements for this highly desirable result are that the fit be least squares and that each J level be weighted by the factor $2J+1$. The use of operators that are orthogonalized in the sense of (2), even in cases where the linearity condition is not rigorously valid, can be expected to lead to parameters p_i whose mean errors are smaller than the usual ones and which can be more accurately extrapolated to unknown spectra.

The conventional operators used in fitting energy levels often do not satisfy (2). For example, the coefficients of F_0 and F_2 in (1) form orthogonal sequences only if the factor $2S_\psi + 1$ is omitted from (2), and this vitiates the extension of the orthogonality concept to d^3 and other d^N configurations. Orthogonality is guaranteed if the product $H_i H_j$ does not contain a part that is scalar with respect to a Lie group for which the states ψ form the basis of a representation. The operators e_0, e_1 and e_2 that Racah used in the f shell are mutually orthogonal because they correspond to different irreducible representations of $O(7)$, which means that no product $e_i e_j$ can contain a component of the scalar transforming like (000) of $O(7)$. By considering other Lie groups such as G_2 , this principle can be extended to include the three-electron operators t_3, t_4, t_6, t_7 , and t_8 with e_0, e_2 , and e_3

in a mutually orthogonal set. Orthogonalization procedures can be developed to replace e_1 , t_2 , and the operators e_α , e_β , and e_γ associated with the three Trees parameters α , β , and γ by other operators that can be included in the set. The advantages and limitations of using orthogonalized operators is discussed for f^3 .

An example of analogous operators for the d shell has already been described¹ for CrIV $3d^3$. An analysis of the mixed configurations $p^N d$ has recently been begun in collaboration with Dr. J. E. Hansen of the Zeeman Laboratory. Orthogonal two-electron scalar operators involving the d electron can be written in the form

$$(p^\dagger_p)^{(\kappa\kappa)} \cdot (d^\dagger_d)^{(\kappa\kappa)},$$

where κ and k define the ranks of the operators in the separate spaces of the p electron and the d electron. The extension to three-electron operators can be written schematically as

$$(p^\dagger_p p^\dagger_p)^{(\kappa\kappa)} \cdot (d^\dagger_d)^{(\kappa\kappa)},$$

but the product of creation and annihilation tensors for the p electron is not precisely defined. In particular, two distinct products can be constructed when $(\kappa\kappa) = (11)$ or (02) . The symplectic group $Sp(6)$, acting in the six-dimensional spin-orbital space of the p electron, is useful here. For both (11) and (02) , the assignment of the irreducible representation $\langle 110 \rangle$ or $\langle 220 \rangle$ of $Sp(6)$ resolves the ambiguities. In addition to 6 two-electron operators, we can construct 11 three-electron operators, all of which are mutually orthogonal. Dr. Hansen is reporting on further aspects of this work at this symposium.

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COMPUTATIONAL SPECTROSCOPY

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The prediction, through computation, of atomic properties pertaining to energy levels and transitions might be viewed as "Computational Spectroscopy." It is useful to distinguish such activities from "theory" since often no new, fundamental theories are developed. Like experimental spectroscopy, computational spectroscopy is a tool for the study of atomic spectra, a tool that still needs considerable refinement. In this paper, several types of calculations will be discussed and progress in computational procedures described.

Often, a fairly simple calculation will suffice to explain the physics of an observed phenomenon, in which case Hartree-Fock calculation might be performed. Though a number of papers have been published that show the importance of term dependence, mainly by Hansen¹⁾, it often is neglected. An example is the interpretation of the 4d - f photoionization spectrum of the isonuclear sequence, Ba, Ba⁺, and Ba²⁺²⁾. It is possible that the average-energy Hartree-Fock calculations have prevailed for so many years because in all MCHF programs³⁾ published to date this was the easiest way of performing the calculations; from the user point of view. For many of the simpler cases, the barrier for a term-dependent calculation has been removed in a new version of an interactive Hartree-Fock program. Limitations on the orbital angular quantum number have been removed and the user may selectively request the display of a number of atomic parameters.

Relativistic effects play an important role in the accurate prediction of transition probabilities for many forbidden transitions. When the atomic systems are highly ionized, the multiconfiguration Dirac-Hartree-Fock method restricted to configurations in the complex, has produced the most reliable results to date.⁴⁾ At lower stages of ionization, where correlation may be more important than purely relativistic effects, the results are not in as good agreement with observation. Several programs, based on the Breit-Pauli approximation, have been developed and used to predict fine-structure splitting. Some typical results for the Oxygen sequence are given in Table 1.

Large scale calculations will be needed to improve the above accuracy. In the Breit-Pauli approximation, the number of configuration states increases rapidly since configurations with several open shells have many couplings. Even so, the configuration expansions are not likely to be as long as those in quantum chemical applications where expansions of length $10^5 - 10^7$ have been reported.

Table 1: Comparison of $2p^4 ({}^3P_0 - {}^3P_2)$ multiconfiguration Breit-Pauli energy separations (in cm^{-1}) in the oxygen sequence with other theory and observation. The values in parentheses in the observed column have been modified to exclude the Lamb shift.

Ion	MCHF + BP ⁵⁾	MCDHF ⁴⁾	Observed ⁶⁾
O	225		227
F ¹⁺	485		490
Ne ²⁺	911	811	921
Mg ⁴⁺	2501	2415	2521
Si ⁶⁺	5526	5452	5568 (5564)
S ⁸⁺	10569	10504	10648 (10640)
Ar ¹⁰⁺	18160	18106	18307 (18293)
Ca ¹²⁺	28892	28590	28880 (28861)
Mn ¹⁷⁺	66731	65711	66505 (64881)
Zn ²²⁺	110273	108544	110437 (107553)

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Parametric Fitting for Low Odd Configurations of U II^{*}

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A single-configuration Hartree-Fock program written by M. Wilson and C. F. Fischer, containing the Cowan-Griffin approximate correction for relativistic effects on the potentials for s electrons¹, is being used to provide estimates of trends for the major interaction integrals in calculations for the untruncated three lowest configurations $5f^3(7s^2+6d7s+6d^2)$ of U II. When experimental data from the U V three-electron configurations $5f^3$ and $5f^2(6d+7s)$ are used to calibrate these corrections, the estimates for the magnetic parameters (but not the electrostatic) can be taken as given in parametric fitting calculations for the more complex U II cases. This greatly simplifies the search for a valid parametric model, since the large mixing of SL basis states, which enhances the chances for false solutions, can be studied in a more controlled way to better match the calculations with experimental g -value, isotope-shift and hyperfine-structure measurements. These results will be briefly discussed, along with the results of a proposal to include in the HF code a correction for relativistic effects on p -electron orbitals as well.

¹R. D. Cowan and D. C. Griffin, J. Opt. Soc. Am. 66, 1010 (1976)^{*}

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PARAMETRIC FITTING TO THE $p^n d$ CONFIGURATIONS USING
A COMPLETE SET OF TWO- AND THREE-BODY PARAMETERS.

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As described in another contribution to this conference we have constructed a complete set of 6 two-body operators and 11 three-body operators which to second order in perturbation theory describe the effect of one- and two-electron excitations on the $p^n d$ configurations. These operators are orthogonal [1] and can be given group theoretical labels. This means, for example, that the parameters have well defined properties under conjugation.

The total number of orthogonal parameters is larger than the number of terms in $p^2 d$. It is equal to the number of terms plus the number of different electrostatic non-diagonal matrix elements which are possible in $p^2 d$. This is different from the situation in a configuration of equivalent electrons. In d^3 , for example, only two three-body operators are linearly independent. Our 11 three-body operators are linearly independent and the number of parameters can only be reduced if some of the parameters have negligible values.

Due to the large number of terms with the same L and S values (but different parents) in $p^2 d$, $p^3 d$ and $p^4 d$, most parameters have non-diagonal matrix elements which means that the energies do not depend linearly on the parameters. In fact due to the conjugation properties mentioned earlier a number of parameters has non-diagonal matrix elements only particularly in $p^3 d$. This makes it difficult to find the values of the parameters by least-squares fitting. The study of the variation in parameter values is further complicated by the fact that the parameters in $p^2 d(p^4 d)$ which have non-diagonal matrix elements only, and therefore are difficult to establish, have diagonal values in $p^3 d$ and vice versa.

We have studied the five $2p^n 3d$ configurations in III, IV and V spectra. Unfortunately, no isoionic sequence seems to exist for which all terms are known in these configurations. Nevertheless good fits have been obtained, particularly in IV spectra, to the pd , $p^2 d$, $p^4 d$ and $p^5 d$ configurations. A fairly large but regular variation of the parameters has been established in preliminary fits. For $p^2 d(p^4 d)$ it is not surprising, given the number of parameters, that a good fit can be obtained but it is somewhat surprising that it so far has been impossible to obtain a good fit to the $p^3 d$ configurations in any of these spectra. However, problems in the fitting to $p^3 d$, even if configuration inter-

action is included explicitly, have been noticed previously by several authors. The problem is still under study.

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POSSIBLE IMPLICATIONS OF THE k ORDERING OF ATOMIC STRUCTURE

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The discovery by the author [1] of a new ordering principle or extended symmetry in atomic physics (characterized by the quantum number k) in 1976 pertains to the excited-state energy spectra of atoms and ions consisting of a single valence electron outside a core of closed shells. The k ordering applies specifically to medium and heavy atoms and ions, i.e., those with atomic number $Z \geq 11$ (Na), so that there is at least one filled p shell in the electron core of the atom or ion. The k -ordering symmetry thus discovered represents in a basic sense the opposite limiting case to the level ordering according to n (n degeneracy) of the hydrogen atom. I have introduced the concepts of the k gross structure, the ℓ semi-fine structure and the associated ℓ patterns. In five recent papers [1-5], I have introduced the concept of the quantum number $k \equiv n + \ell$ as an energy-ordering quantum number for the excited-state energy levels of the neutral alkali-metal atoms and the singly ionized alkaline-earth atoms and, in addition, pseudo-one-electron states in the Group IB, IIA, IIB and IIIA elements of the Periodic Table. Except in a few cases, the ℓ pattern does not change with increasing k , and as an outstanding example, the ℓ pattern is pdsf for a total of 158 excited states of rubidium extending from $k=6$ to $k=55$ [6].

In view of the wide prevalence of the phenomenon of k ordering (1400-1500 levels), it is likely that the underlying effect is a very fundamental one and is the expression of a very basic aspect of atomic structure which has not been incorporated in the present descriptions of atomic energy levels. These descriptions belong to two types: (1) the calculation of the energy levels by means of a suitable "realistic" effective one-electron potential $V(r)$ which approaches $-2Z/r$ (Ry) near the nucleus and $-2(1+Z-N)/r$ (Ry) at large radii r ; (2) the modification of the Rydberg formula for a hydrogenic atom by the inclusion of a suitable quantum defect $\delta_{n\ell}$. In the course of my calculations of the Sternheimer antishielding factors [7] γ_∞ and R , and of the electronic polarizabilities [8] α_d and α_q , and in earlier calculations [9], I have had extensive experience with the solution of the radial Schrödinger equation using a wide variety of potentials, and in my opinion, it would be nearly miraculous to reproduce accurately the small energy differences (sometimes only of the order of 1 meV) between states with different values of both ℓ and n . The relation of the curve of $\delta_{n\ell}$ vs ℓ to the k ordering has been examined in Ref. 5. Possible explanations of the observed k ordering of atomic and ionic energy levels have been proposed by Sternheimer [4] (in terms of a basic k -symmetry breaking) and by Foley [10], Ostrovsky [11], and Armstrong [12].

As an additional confirmation of the existence of the k ordering, we consider the values of the mean excitation potential I which enters into the Bethe-Bloch formula for the ionization loss dE/dx of charged particles

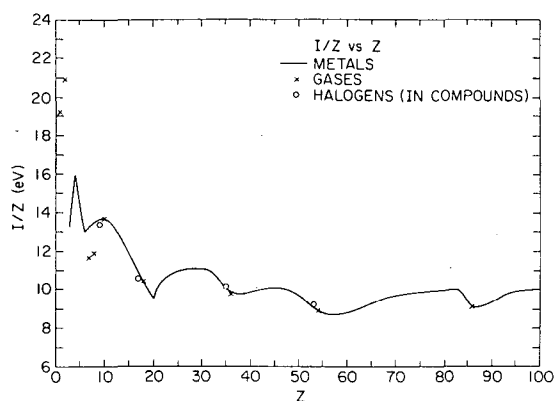


FIG. 1. Values of I/Z (in units eV) plotted as a function of the atomic number Z . Here I is the mean excitation potential of the substance. The smooth curve passes through the values of I/Z for the elemental substances (metals) as determined by Berger and Seltzer. The crosses correspond to the values of I/Z for gases; the open circles indicate the values of I/Z used for halogens in compounds.

[13]. When I/Z is plotted against Z , the resulting curve has successive maxima and minima as shown in the Figure. The local minima of I/Z at $Z=6$, 20, 56, and 86 correspond respectively to the filling of the $2p^6$ shell (carbon), the completion of $3p^6 4s^2$ (Ca), $4p^6 5s^2$ (Sr), $4d^{10} 5p^6 6s^2$ (Ba) and $4f^{14} 5d^{10} 6p^6$ (Rn). It is of interest that the minima of the I/Z vs Z curve coincide approximately with the closing of the successive k -supershells of the Periodic Table, as defined in Ref. 1. The present work was supported by the U. S. Department of Energy under Contract No. DE-AC02-76CH00016.

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Matrix Elements for Spin-Dependent Interactions
in $\ell \ell'$ Configurations

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Formulas for the matrix elements of the two-electron spin-dependent interactions: spin-spin, spin-other-orbit, and effective electrostatic-spin orbit (EL-SO), were constructed for $\ell \ell'$ configurations.

Twelve angular momenta participate in the orbital part of each of these matrix elements. In the direct part of each interaction, these angular momenta are connected according to the identity of Arima, Horie and Tanabe⁽¹⁾:

$$\sum_{xy} [x][y] (-1)^{y - j_2 + j'_1 + j'_2 - j - k - k_1 + \ell_2}$$

$$\left\{ \begin{matrix} j & j_2 & j'_1 \\ j'_2 & j'_1 & j'_1 \\ k & x & y \end{matrix} \right\} = \left\{ \begin{matrix} \ell_2 & \ell_1 & j \\ j_2 & j_1 & j' \\ j_1 & j_2 & k' \end{matrix} \right\}$$

In the exchange part of each of these interactions, all orbital angular momenta are grouped in a 12j-symbol of the first kind, according to the following new identity:

$$\sum_{xy} [x][y] (-1)^{2y + j + j' + j_2 - j_1 + k_1 + k_2 + \ell_1 - \ell_2}$$

$$\left\{ \begin{matrix} j & j_2 & j'_1 \\ j'_2 & j'_1 & j'_1 \\ k & x & y \end{matrix} \right\} = \left\{ \begin{matrix} j_1 & j' & j & j_2 \\ & j'_2 & k & j'_1 & k' \\ \ell_2 & k_2 & k_1 & \ell_1 \end{matrix} \right\}$$

The well known formulas for the electrostatic interaction in $\ell \ell'$ configurations are, of course, obtained on using the above identities, with $k = 0$.

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These identities are also useful in simplifying formulas of matrix elements of additional interactions, the tensor-operator form of which includes irreducible products of orbital operators with rank $k \neq 0$; for instance, the 3-electron electrostatic effective interaction in $\ell^N \ell'$ configurations.

**THEORY, ION TRAPS,
AND LASER COOLING**

ArII - ArXVI produced in slow recoil collisions

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An atom in a gaseous target may be highly ionized in a single collision with a (very fast) very highly ionized projectile. A feature of the kinematics of the collision is that very little kinetic energy is imparted to the target atom. The ion is produced as a slow recoil. Typical recoil energies are 1 eV and change little with the degree of ionization produced in the target. This has several very attractive features as a spectroscopic source. First, the spectra are free from Doppler shifts which depend upon the degree of ionization of the atom, and, second, all of the ionization states produced in the target have the same spatial distribution. This allows reference lines from low ionization states to be reliably used to calibrate the spectra from high ionization states.

Argon gas at pressures of 0.02 to 1.0 Torr was bombarded with a variety of projectiles obtained from the Lawrence Berkeley Laboratory's Super-HILAC. The projectiles had average ionization states ranging from 16+ for argon projectiles to >55+ for uranium. Spectra were observed in the 15 nm - 70 nm region using a 2.2 m grazing-incidence spectrograph (McPherson model 247) with a 300 groove/mm grating and a two-dimensional microchannel-plate detector. In later experiments Kodak type 101-05 photographic plates were used in place of the microchannel-plate detector.

The microchannel-plate detector was used to compare the relative cross sections for producing spectra by different projectiles and to determine initial values for the beam energy, target pressure, and minimum exposure time for photographic plates. Beams of Fe, Xe, and Au at energies of 4.6 MeV/nucleon were then used for experiments with photographic plates. The experiment which produced spectra from the highest charge state of argon utilized a Au beam (average charge state of 53+). After a 40 hour exposure to a 1 torr Ar target bombarded by the Au beam (integrated beam current = 675 particle μ A seconds), over 400 first- and second- order argon lines were observed in the 15 nm - 70 nm region of the plate. A preliminary analysis has identified lines from ArII - ArVIII, ArX - ArXIV, and the $2^2P_{3/2,1/2} - 2^2S_{1/2}$ doublet in ArXVI. Comparison of the spectra with spectra produced by bombarding argon with Xe and Fe beams has so far failed to show any lines which arise from the projectiles.

I thank Mr. Douglas MacDonald, Dr. Daniel Dietrich and Mr. Charles Munger for their assistance and Prof. Richard Marrus for his support and encouragement. I am especially grateful to the operators and staff of the Super-HILAC who willingly try the impossible- and often succeed. This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Chemical Sciences Division, U.S. Department of Energy, under Contract No. DE-AC-03-76SF00098.

LASER COOLING OF AN ATOMIC BEAM WITH FREQUENCY-SWEEP TECHNIQUES

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We discuss an experimental scheme for velocity-modifying an atomic beam by scattering of intense light from a frequency-swept laser source. This technique, capable of working at almost zero magnetic field, is substantially supported by a new rf/optical modulation method to generate the desired profiles of laser optical frequency and intensity versus time. This digital method provides the necessary sweep accuracy and program flexibility in a convenient and powerful way. First experiments velocity-modifying a sodium atomic beam are in preparation and can directly be compared with recent similar experiments at NBS [1]. First results will be presented if available.

The second topic of this paper is a Monte Carlo simulation program which provides useful insights into the system behavior, aids in the design of the actual atomic beam apparatus, and offers a channel for comparison of the experimental results with theory. This simulation program takes into account all necessary effects as e.g. random emission times, optical pumping, and transverse heating. The results of these calculations for a sodium atomic beam (initial collimation of 3 mrad) indicate the possibility of an average longitudinal velocity of zero with a residual width (at half maximum) of ~ 3 m/s in longitudinal direction and 8 m/s or less in transverse directions.

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LASER COOLING AND ION FREQUENCY STANDARDS

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Ions which are stored in electromagnetic traps provide the basis for performing high resolution spectroscopy where systematic frequency shifts can be quite small. For many years, the largest uncertainty in such experiments has been due to Doppler effects caused by the ion motion. Using radiation pressure from lasers, the kinetic energy of stored ions can now be reduced to temperatures significantly less than 1K thereby greatly suppressing Doppler frequency shifts. Experiments now in progress suggest spectroscopic inaccuracy less than 1 part in 10^{15} with application to frequency standards and clocks.

FORBIDDEN SPECTRA AND DECAY RATES FROM METASTABLE TRAPPED IONS

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An ion trap containing a number of metastable excited ions can be regarded as a light source from which only forbidden radiation is emitted. Nearly always, the excitation process is short compared to the confinement time which is much longer than allowed decay lifetimes. Thus, after the pulsed excitation and a brief (say 1 μ sec) period thereafter, only ions in the ground state or long lived (metastable) excited states are present in the storage volume. Since ions can be confined for long periods (up to many hours) without significant loss, the possibility exists of observing a forbidden emission spectrum in the absence of a far more intense allowed spectrum. Furthermore, in most cases, measurement of the decay of a given forbidden line gives directly the lifetime of the metastable level from which it arises. This latter ability to measure metastable lifetimes has been applied successfully in the past^{1,2} to one and two electron ions, where only a single decay was important and spectral resolution by the radiation detector was not required. In more complex ions, however, the forbidden spectrum can be quite dense and meaningful lifetime measurements for the different excited levels will require varying degrees of spectral resolution in the detection channel. For a spectrum with well separated lines (more than about 10 Angstroms apart), one can use appropriate interference filters to isolate the line of interest (see for example the work of R.D. Knight³). A more flexible system uses a small dispersive spectrometer, which allows collection of a low resolution spectrum, and with modern position sensitive detectors, parallel collection of the decay of many lines.

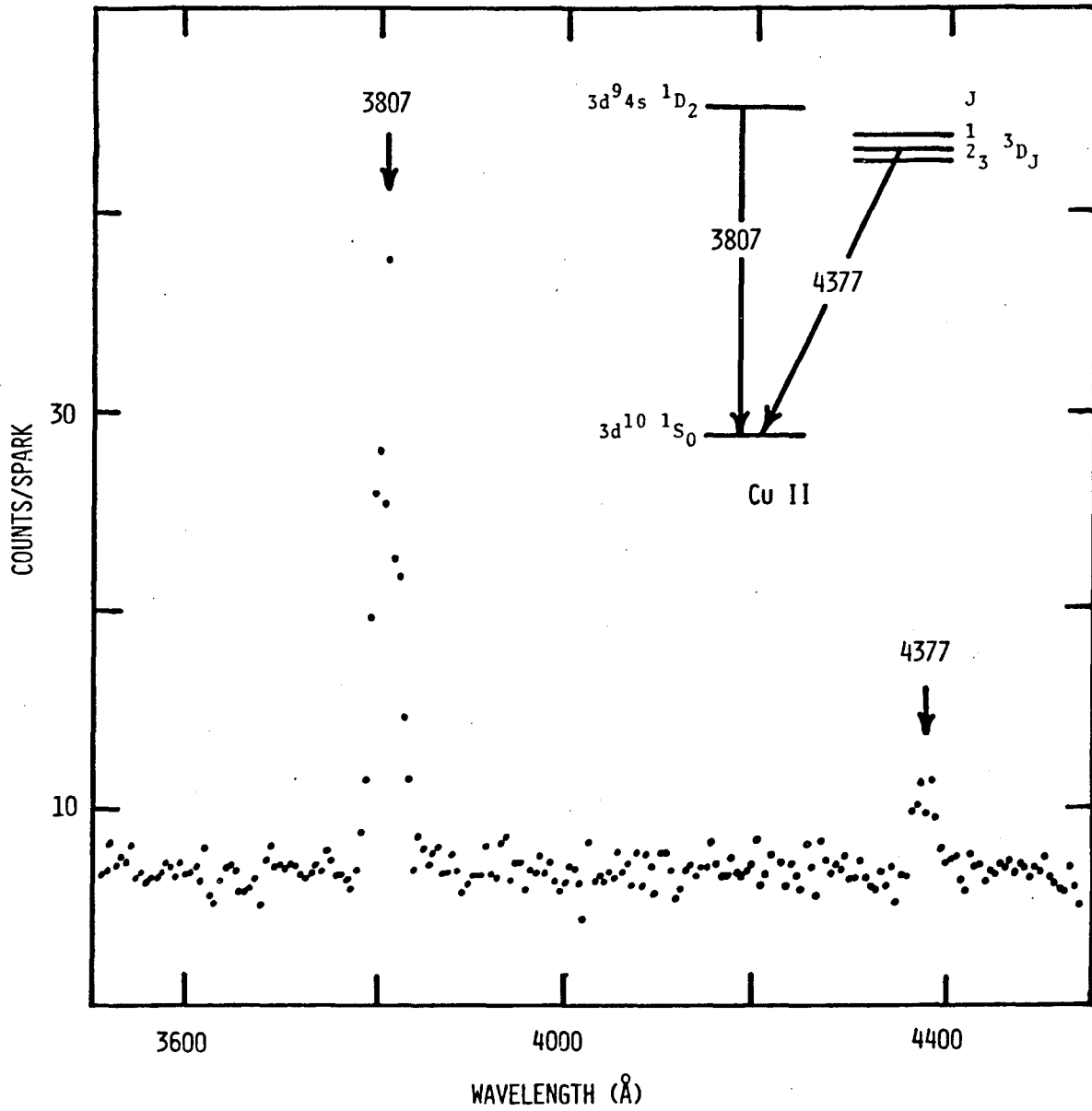
The work reported here gives examples of the study of electric quadrupole (E2) decay from metastable CuII ions in the $3d^9 4s^1 D_2$ and 3D_2 states, and mixed E2 and magnetic dipole (M1) decay from $3p^4 1S_0$, ArIII ions. In both cases the ions were confined in simple electrostatic ion traps and the radiation dispersed by a 1/4 m Ebert monochromator. The CuII ions were produced by a vacuum spark discharge external to the ion trap, whereas the ArIII ions were made inside the trap by electron impact. An example of the CuII forbidden line spectrum is shown in the figure.

Details of the experimental technique and examples of decay curves for the forbidden line intensities will be presented. Measured values of the upper state lifetimes will be reported and compared with theoretical predictions. Prospects for precision spectroscopy of forbidden lines of trapped ions will be discussed if time allows.

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E2 lines from trapped metastable CuII ions. The A value for the 3807 line is about 2 per second.

Two- and Three-Electron Effective Electrostatic Interactions
in the $3d^N 4p$ Configurations of the Third and Fourth
Spectra of the Iron Group.

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A complete set of two- and three-electron effective electrostatic interactions among d electrons as well as among d and p electrons were included in the energy matrices of the $d^N p$ configurations.

A systematic investigation was conducted on the effects of the above mentioned interactions on the energy level structure of the $3d^N 4p$ configurations of the third and fourth spectra of the iron group.

The inclusion of these interactions greatly improved the fit between observed and calculated energy levels. For example, a general-least-squares (GLS) calculation of the fourth iron group spectra resulted in a mean error of 104 cm^{-1} when, in addition to the effective core parameters α , β , T and Tx, the d-p two-electron effective parameters F_1 and G_2 were included. Furthermore, on adding the d-d-p three-electron effective parameters, the mean error reduced to 39 cm^{-1} .

Consistent values were obtained for the various interaction parameters, and their variations, both along an isoionic sequence and for different ions of the same element were determined. For all configurations, the values of the "real" Slater and the spin-orbit parameters were also calculated by using the Hartree-Fock method, and compared with the corresponding semi-empirical values.

Spin-Dependent Interactions in the $3d^N$ Configurations
of the Fourth and Fifth Spectra of the Iron Group.

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A systematic investigation was conducted on the effects of spin-dependent interactions on the energy level schemes of the $3d^N$ configurations ($N=2,3,\dots,8$) in the fourth and fifth spectra of the iron group. The spin-dependent interactions considered were the spin-spin, the spin-other-orbit and the effective electrostatic-spin orbit (EL-SO) interactions.

The values of the appropriate radial integrals $M^k(k=0,2)$ and $Q^k(k=2,4)$ were determined by using both ab-initio and semi-empirical methods.

In the semi-empirical method, the introduction of the spin-dependent interactions greatly improved the fit between calculated and observed multiplet splittings in all investigated configurations. Consistent values were obtained for the various parameters, which agree very well with those obtained in the ab-initio calculations.

The variations of the parameters, both along an iso-ionic sequence and with the degree of ionization of the same element, were determined.

CONFIGURATION INTERACTIONS IN THE Fe I AND Co I
SEQUENCES IN THE IONS OF THE ELEMENTS As, Se AND Br.

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In the Fe I isoelectronic sequence analyses of Sr XIII - Ag XXII [1,2] and Zn V [3] have been published recently.

From Hartree-Fock calculations it can be concluded that in the sequence Fe I - Ge VII the separation between the $3d^7 4p$ and $3p^5 3d^9$ configurations is so large that configuration interaction can be neglected. In these spectra the $3d^7 4p$ configuration is the lowest one whereas from Kr XI it is just the opposite.

In As VIII, Se IX and Br X strong interaction is present between these configurations; perturbations of levels between 1000 cm^{-1} and 10.000 cm^{-1} have been observed. In these spectra all levels of the ground configuration ($3d^8$) and most of the levels of the odd configurations have been determined.

In the Co I isoelectronic sequence our investigation reveals that the configuration interaction between the $3d^8 4f$ configuration and $3p^5 3d^{10}$ is much stronger than between the $3d^8 5p$ configuration in As VII, Se VIII and Br IX. This is contrary to Zapriagaev et al. [4] has found in Se VIII.

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BEAM FOIL

Invited Speaker

BEAM FOIL SPECTROSCOPY

Ove Poulsen

University of Aarhus

Invited Speaker

FAST-ION SPECTROSCOPY OF HIGHLY IONIZED ATOMS

A. E. Livingston

University of Notre Dame

Application of the parametric description of the isotope
shift (PADIS) to the lanthanides

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Recently /1/ we have shown that the parametric description of the isotope shift (PADIS) - according to /2/ - is very useful in the series of the 5d-elements. Especially for the elements W through Pt systematic trends of the parameters of PADIS are obvious /1/. This is caused by the fact, that the low-lying configurations $(5d + 6s)^n$ lie close together in the finestructure scheme and are well separated from disturbing higher configurations. Therefore, the wavefunctions in intermediate coupling are known with sufficient accuracy. This makes a parametric description of the IS possible for practically all levels of configurations of the type $(5d + 6s)^n$.

In the lanthanides, however, normally strong configuration interactions exist which result in only rough estimates of the wavefunctions. But

- (i) some multiplet terms in the low-lying configurations $(4f^{n-2}6s^2, 4f^{n-1}6s, 4f^{n-3}5d6s^2, 4f^{n-2}5d6s)$ and
- (ii) only in a few lanthanide elements complete excited configurations of the type $4f^{n-2}6s6p$

are known which are sufficiently unperturbed. Therefore, it seemed interesting to us also for the series of the lanthanides to start systematic investigations of the IS of those selected multiplet terms and configurations and to describe the IS with PADIS.

For the case (i), i.e. the IS-investigation of individual multiplets, only the J-dependence of the IS described by the "crossed-second-order" parameter z_{4f} or z_{5d} can be evaluated. The results known so far are compiled in table I and will be discussed.

In the analysis of whole configurations (case (ii)), however, the complete set of IS parameters can be achieved.

As a first suitable example we chose the rather "pure" Eu-I configuration $4f^7(8S_{7/2})6s6p$. The completion of the hyperfine structure of this configuration (twelve levels) we investigated the levels $z^6P_{3/2}$ and $z^{10}P_{7/2, 9/2, 11/2}$. For the analysis even two different finestructure calculations - namely by /3/ with three mixing configurations, and by /4/ with seven mixing configurations - were at our disposal. From our calculations - which will be discussed in detail - first and second order IS-parameters could be achieved which are compiled in table II.

Further results and aspects of the applicability of the parametric description to other lanthanides will also be discussed.

Element	Configuration/Multiplet	z_{nl} (mK)	Author
Sm ¹⁴⁴⁻¹⁵² I	$4f^6 6s^2$ 7F	1,68 (30)	/5/
Eu ¹⁵¹⁻¹⁵³ I	$4f^7 5d6s$ ^{10}D	1,53 (20)	/6/
	8D	1,67 (87)	/7/
Dy ¹⁶⁰⁻¹⁶⁴ II	$4f^{10} 6s$ 6I	1,09 (22)	/8/

Table I: "Crossed-second-order" parameter z_{4f} and z_{5d}

a	= - 130(4)	mK
g_1	= - 4(4)	mK
z_{6p}	= 0(0,5)	mK
g_3	= - 0,70(11)	mK

Table II: IS₂ parameters of $4f^7 6s6p$ in Eu-I

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The Use of Hyperfine Structures in the Analysis of the Americium I Spectrum

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The analysis of rare earth spectra has always been a great challenge due to the high density of spectral lines. The spectrum of americium has attracted interest since the 5f core is half filled and effectively contributes only a single parent. Thus the spectrum of americium is simpler than the spectrum of any of its neighbors. The analysis of the spectrum, though, has been hampered by the broad hyperfine structure of most of the spectral lines. These lines overlap and make the use of automatic peak-finding programs impractical. Extensive measurements of the spectrum have been previously made by M. Fred and F. S. Tomkins(1). The data used in the present analysis were taken by F. S. Tomkins and J. Brault using the solar laboratory fourier spectrometer at Kitt Peak Observatory.

The presence of hyperfine structure in spectral lines has been considered by many investigators to be a hinderance to the accurate determination of atomic energy levels. Peak-finding techniques are of limited value because the peak is not at the center of gravity of the line. Center-of-gravity techniques can be difficult with imperfect knowledge of the extent of the hyperfine structure. Computer programs were developed by the author while he was at Purdue University which are capable of handling a broad range of fully and partially resolved hyperfine patterns. These programs perform a nonlinear-least-squares fit of the data to a theoretical model. The result of this fit is not only an accurate center of gravity for the spectral line but also a determination of the J quantum number and A and B splitting factors of the combining levels.

The analysis of the americium spectrum is further complicated by the extensive overlapping of spectral lines. We have modified our computer programs to allow the fitting of up to three overlapping spectral lines simultaneously. When a known and unknown spectral line overlap, the program can make use of previous measurements to generate the profile of the known spectral line and subtract it from the data to obtain that of the unknown line. Another complication that has been found in the americium spectrum is that some of the transitions to the ground state are self-reversed. We have modified our program to utilize the expected self-reversed profiles(2) in these cases.

Due to the overlapping lines in the americium spectrum, as many levels as possible are first being determined by hyperfine measurements before a complete and careful measurement of the spectrum is made. The method used is to first very quickly and roughly measure the center of gravities of the spectral lines using an interactive line-finding computer program written by Craig Sansonetti.

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The resulting wavenumbers are then fed to a level-finding program which determines possible new energy levels using previously determined levels. Each possible new level is checked by analyzing the hyperfine structure of a spectral line involved in that level. If the J value and splitting factors of the known level do not agree with previously measured values then the tentative new level is discarded. If they do agree then a second spectral line is checked. If the J values and splitting factors of both the known level and the tentative level agree with previous measurements then the tentative level can be accepted as a new level with high certainty. Using this technique over 150 new levels were quickly discovered.

A complete analysis of the americium spectrum would be nearly impossible without the aid of the hyperfine structure analysis. This preliminary investigation has already accurately located over 200 energy levels. Very little has been done with the configuration analysis and it is expected that this will remain a difficult problem well after most energy levels have been located. However, the J values and splitting factors determined by this investigation should help in this endeavor. Our hyperfine structure analysis techniques are being extended so that they can be used on photographic data. This will greatly increase the wealth of information available.

Configuration interaction in the hyperfine structure
of transition elements

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The study of configuration interaction (CI) in multi-electron atoms by high-precision hyperfine structure (hfs) measurements is still a challenge to atomic spectroscopy mainly for two reasons: 1) In order to obtain reliable information on CI that can be compared with ab initio calculations the hfs has to be measured in many atomic states of the same configuration. Substantial experimental and theoretical progress has been made in recent years, but there are a number of areas in need of additional work. 2) For the accurate determination of nuclear properties such as nuclear moments or the distribution of nuclear magnetism from the hfs one has to know precise values of the electronic part of the hyperfine interaction including effects of relativity and CI.

An ideal field for a detailed study of CI effects in the hfs which is also of particular interest from the standpoint of nuclear physics are the transition elements with an unfilled 4d or 5d electron shell, because these elements have many metastable states belonging to the configurations nd^N , $nd^{N-1}(n+1)s$, and $nd^{N-2}(n+1)s^2$, which can be investigated by high precision radio-frequency (rf) spectroscopy.

Therefore, in order to study CI effects in these atoms we measured the hfs of many metastable states of 4d- and 5d-shell atoms using the atomic beam magnetic resonance technique. Atomic beams of these refractory elements were produced crucible-free using the rotating-target method /1/. The magnetic field region of the apparatus is conventionally equipped with two-pole inhomogeneous deflecting magnets for flop-in detection of rf transitions induced in the homogeneous C-magnet. The rf resonant atoms were detected either by electron bombardment ionization and subsequent mass separation or by a state- and isotope-selective laser detection scheme /2/.

The experimental hfs data were analyzed with respect to the effective operator formalism /3/ yielding values of the effective hfs parameters a^{ij} ($ij=01,12,10$) for the magnetic dipole and b^{ij} ($ij=02,13,11$) for the electric quadrupole interaction, which take into account both relativistic and CI effects on the hfs. Using known values of the nuclear dipole and quadrupole

moments the associated $\langle r^{-3} \rangle$ radial integrals were evaluated.

In order to obtain an estimate of the effects of CI relativistic $\langle r^{-3} \rangle$ radial integrals were evaluated from relativistic self-consistent field radial wavefunctions. The wavefunctions were calculated by using the atomic multiconfiguration Dirac-Fock program developed by Grant et al. /4/. For averaging over all the jj subconfigurations arising from the entire SL configurations the extended average level method /4/ has been applied.

The comparison of the experimental $\langle r^{-3} \rangle$ values with the theoretical values clearly indicates a strong influence of CI on the hfs of the 4d- and 5d-atoms. In particular, for the radial integrals $\langle r^{-3} \rangle^{12}$ and $\langle r^{-3} \rangle^{10}$ of the magnetic dipole and the integral $\langle r^{-3} \rangle^{02}$ of the electric quadrupole interaction a systematic deviation of the experimental values from the relativistic ones could be established.

Although the effective operator formalism works fairly well for the investigated complex atoms, in most cases the hfs constants cannot be reproduced exactly within the experimental limits of error. These remaining discrepancies are probably due to electrostatically correlated second order hfs effects, which lead to SL-dependent effective hfs parameters /5/.

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EFFECTS OF NUCLEAR STRUCTURE IN THE $1s2s\ ^3S_1$ HYPERFINE SPLITTINGS OF HELIUM-LIKE $^{6,7}\text{Li}^+$ IONS

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Significant nuclear structure effects are exhibited in the atomic hyperfine structure (hfs) due to the finite distribution of nuclear charge and magnetism. This manifests itself e.g. in the hyperfine anomaly which is defined for a pair of isotopes as $^{1,2}\Delta = 1 - (A_{\text{exp}}^2/A_{\text{exp}}^1)(g_I^1/g_I^2)(M^*/M^*)$. In this formula A_{exp} is the magnetic dipole hfs interaction constant, g_I the experimental nuclear gyromagnetic ratio, attributed to a point-like nucleus, and $M^* = (1+m_e/M_{\text{nuc}})^{-3}$ a reduced-mass factor. The comparison between experimental and theoretical anomaly data provided valuable information on the validity of the applied model in the case of many heavy nuclei. A review has been given by H.M. Foley¹. For a single isotope, A_{exp} can be related to a theoretical value A_{cal} , representing a point-like nucleus via the equation $A_{\text{exp}} = A_{\text{cal}}(1 + \Delta_{\text{nuc}})$. Presently it is not possible to calculate a hfs splitting energy of a many-electron atom with sufficient accuracy in order to isolate the small fraction $\Delta_{\text{nuc}} = \Delta$ arising from the nuclear structure. However, A_{cal} can be calculated accurately for one- and two-electron atoms, since precise nonrelativistic wave functions as well as relativistic and QED correction factors are available. Thus the A-factors of the $1s^2S_{1/2}$ ground state and metastable $2s\ ^2S_{1/2}$ state of hydrogen, deuterium, tritium and $^3\text{He}^+$, and of the metastable $1s2s\ ^3S_1$ state of ^3He have been measured with great accuracy using microwave techniques (see e.g. ref.2) and by comparison with calculated values, provided the nuclear structure effects Δ for the single nuclei. Detailed theoretical studies dealt with the interpretation of the various Δ (see e.g. ref.3).

In this contribution, experimental values of Δ are presented for ^6Li and ^7Li . They have been obtained with combined laser-microwave spectroscopy^{4,5} of the metastable $1s2s\ ^3S_1$ hfs multiplet of helium-like $^{6,7}\text{Li}^+$. In the $2\ ^3S_1$ state the magnetic hfs constant A arises exclusively from Fermi contact interaction between electron spins and nuclear spin and can be expressed by the formula

$$A(2^3S_1)_{\text{exp}} = 36\alpha^2(g_I/\mu_N)(m_e/m_p)R_\infty \text{ cm}^* [1+\delta_{\text{rel}}(1s)+\delta_{\text{qed}}(1s) + \delta_{M,\text{rel}} + \epsilon(1+\delta_{\text{rel}}(2s) + \delta_{\text{qed}}(2s) + \delta_{M,\text{rel}})](1+\Delta_{\text{nuc}}) = A_{\text{cal}}(1+\Delta_{\text{nuc}}).$$

The terms in brackets represent relativistic (δ_{rel} ; $\delta_{M,\text{rel}}$) and radiative (δ_{qed}) corrections as well as a correction for the presence of the 2s electron (ϵ). Evaluation for each isotope with the most precise fundamental constants and correction data, available in the literature, lead to explicit values for ${}^6\Delta$ and ${}^7\Delta$. If all numbers in the above equation equal for both isotopes are comprised in a factor C, the ratio

$$\frac{{}^7A_{\text{exp}}}{{}^6A_{\text{exp}}} = \frac{C^7 g_I \cdot {}^7M^*(1+{}^7\Delta)}{C^6 g_I \cdot {}^6M^*(1+{}^6\Delta)} \text{ transforms to } \frac{{}^7A_{\text{exp}} g_I {}^6M^*}{{}^6A_{\text{exp}} g_I {}^7M^*} = \frac{1+{}^7\Delta}{1+{}^6\Delta} \approx 1+{}^7\Delta-{}^6\Delta = 1-{}^6,{}^7\Delta.$$

This equation illustrates the connection between hyperfine anomaly and nuclear structure effects of single isotopes. Therefore taking ${}^7,{}^8\Delta$ from ref.6 allowed us also to calculate ${}^8\Delta$. Table 1 contains the experimental Δ of H,D,T, ${}^3\text{He}$, ${}^6\text{Li}$, ${}^7\text{Li}$ and ${}^8\text{Li}$ together with the existing respective theoretical data.

Table 1 Exp. and theor. Δ_{nuc} (in ppm) available for single isotopes

	H	D#	T#	${}^3\text{He}$	${}^6\text{Li}\S$	${}^7\text{Li}\S$	${}^8\text{Li}\S$
Exp.	-33(3)	+170.3(0.5)	-5.7(0.2)	-186(9)	-276(30)	-383(30)	-307(36)
Theor.	-33(3)	+195 (41)	+17 (2)	-(160-200)	--	--	--

\S This work. The errors are partly based on the assumption, that δ_{rel} and δ_{qed} produce an uncertainty upon A_{cal} of 2×10^{-5} .

\# The data of D and T, as taken from the literature (see ref.1), are hyperfine anomalies with respect to H.

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Beam-Foil Study of Titanium in the EUV and Population of
Yrast levels

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The ultraviolet spectrum ($8 \text{ nm} < \lambda < 60 \text{ nm}$) of highly ionized titanium after foil excitation of 15 MeV and 20 MeV fast ions has been recorded. A number of new lines, mainly in sodium-like Ti XII, has been identified.

Line intensity ratios are determined making use of the relative calibration of the Bochum spectrometer. Decay curves are measured for the Ti XII levels 3p, 4f, and 5g, and compared with simulated curves assuming different population laws for states up to $n = 20$. Little evidence is found for an overpopulation of yrast states near $n = 15$ as suggested by the resonance mechanism proposed by Veje [1] and Winter et al. [2]. This model seems to reproduce the measurements on Na I-like Ar VIII at 2 MeV beam energy [3], but may not be applicable to the system and energy range studied here.

The use of different materials as exciter foils did not produce significant changes of line intensity ratios or 4f and 5g decay curves. In some cases, however, low- n states are less populated than with pure carbon foils, while in the range $8 \lesssim n \lesssim 16$ the populations seem to be independent of the foil material. This suggests that the high- n , high- l population occurs at the last surface layer which consists of similar impurities on the surface of all foils.

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417 (1981)

POSTERS

TRANSITION PROBABILITIES FOR FORBIDDEN LINES:
THE SILICON ISOELECTRONIC SEQUENCE FROM S III TO SN XXXVII

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Summary

New calculations of transition probabilities for all the $3p^2$ forbidden lines, for alternate ions from S III to Sn XXXVII are presented and discussed. Radial wavefunctions and energy levels were calculated for the $3p^2$ and five low interacting configurations using the HXR self-consistent-field method and Slater-Condon theory. Detailed relativistic corrections and configuration mixing effects were included. Wavelengths and A-values were computed in intermediate coupling with Z-smoothed semi-empirical coupling transformations. Results agree well with those of Mendoza and Zeippen (1982) who used a very different model, and confirm significant improvements over earlier published A-values. The present results extend the data to zinc and beyond to $Z=50$, thus better illustrating trends in magnetic dipole and electric quadrupole oscillator strengths with Z .

(x) Research Associate of the Belgian National Fund for Scientific Research (FNRS)

The Need for Complete Assignments of
All Low-Lying Atomic Levels for Thermodynamic Calculations

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To accurately calculate the thermodynamic properties of the gaseous atoms to temperatures as high as 3000K, it is necessary to know all low-lying electronic levels up to at least 17000 cm^{-1} and preferably to 18000 cm^{-1} . For a number of the transition metals and for most of the lanthanides and actinides, the available assignments of observed levels do not account for all of the expected low lying levels.

To remedy this lack of complete assignments, help has been solicited from atomic spectroscopists who might have unreported values which would extend the listings of low-lying levels. Also unpublished calculations have been located which can provide energy values of sufficient accuracy for unreported levels. Finally, various predictive models have been used to fill in energies of still missing levels.

These supplements have improved the situation so that for all but half a dozen of the elements from hydrogen to lawrencium, the limiting accuracy for temperatures below 3000K is set by the uncertainty of the atomic weights and of the Boltzmann constant. For a number of elements, the uncertainty in $-(G^\circ - H_{298}^\circ)/RT$ at 3000K is as low as 0.0001. The calculated values have been fit to analytical equations which provide values of $-(G^\circ - H_{298}^\circ)/RT$ as a function of temperature.

This work was supported by the Division of
Materials Sciences, Office of Basic Energy
Sciences, U.S. Department of Energy, under
Contract DE-AC03-76SF00098.

Conversion of a Plane Grating Spectrometer into a
Concave Grating Spectrometer for the Far Ultraviolet

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Attenuation by the four reflections internal to our 2 meter Czerny-Turner spectrometer made it impossible to record any but the strongest lines below 1500 Å. Utilizing only the vacuum chamber and grating drive of the plane grating instrument, we converted it to use a 2.18 meter concave grating. A vacuum extension was constructed containing a plate holder machined to fit the Rowland circle, which could be rotated about the entrance slit. Most alignment was made in the zeroth order, with corrections to the grating angle determined from known ultraviolet lines. No other corrections were required to photographically record uniformly sharp and symmetric spectral lines between 2000 Å and 1130 Å using calculated settings.

Spectra from a hollow-cathode lamp included all previously known Pb II vacuum ultraviolet lines down to 1144 Å, below which the magnesium fluoride window of the light source blocked all radiation. Copper added to the cathode provided internal Cu II standards which made it possible to measure the Pb II lines with accuracies of about ± 0.01 Å.

On the Dependency of the Free Spectral Range of a
Fabry-Perot-Interferometer on Mirror-Design, Wavenumber and
Scanning-Pressure

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Since multilayer dielectric mirrors are for more than 30 years normally used to build up a Fabry-Perot-interferometer (FPI) the resolution and luminosity, and therefore the applicability and accuracy of this spectroscopic instrument could be highly increased.

For both dielectric and metal-film mirrors the apparatus-function (Airy-formula) is the same.

But in practical work it was often overlooked or at least neglected that the thickness of a dielectric mirror may extend up to $2 \mu\text{m}$, equivalent to several wavelengths, whereas the thickness of a metal-mirror (only about $1/10$ of a wavelength) could safely be neglected in all practical cases for the calculation of the "Free Spectral Range" ($\text{FSR} = 1 / (2 * n * d)$, with n being the refractive index within the spacer of thickness d).

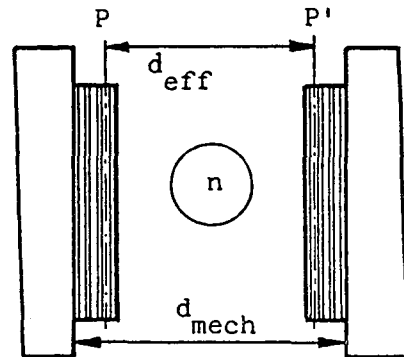
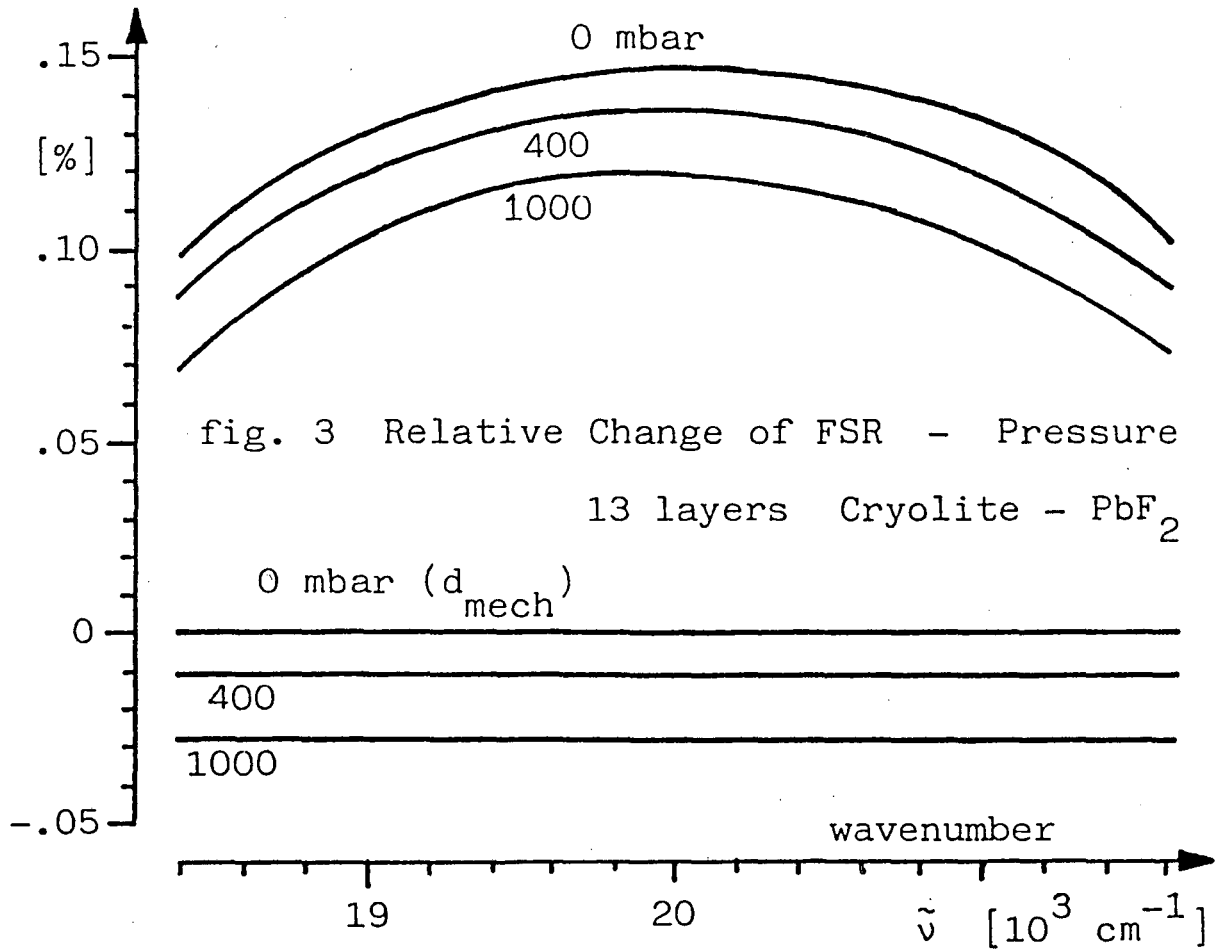
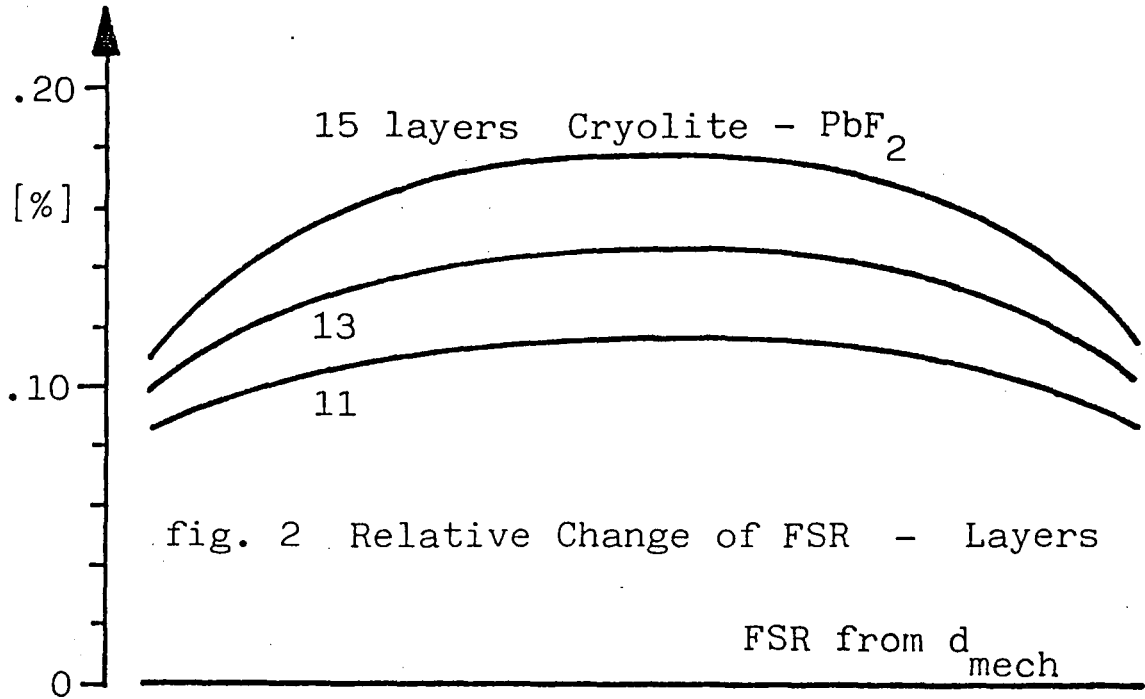


fig. 1 Scheme of a
Multilayer FPI

In the case of dielectric mirrors, however, the surface of the mirror-plates and the effective planes of reflectance (P, P' in fig. 1) are no longer identical, so that with small etalon-spacers (1 mm or even less) the thickness of the two mirrors together easily reaches the range of one or a few tenths of a percent of the spacer and the FSR will be correspondingly wrong. This is detrimental, since in almost all spectroscopic experiments the FSR is used to calibrate the wavenumber-axis by relating the recorded spectroscopic structure to units of an FSR. Thus any uncertainty of the FSR directly leads to an uncertainty of the complete analysis.

Up to now the positions of the "Effective Planes of Reflectance" of a dielectric mirror were not accurately known. We therefore carried out calculations determining them by considering a complete FPI as one set of dielectric layers which can be treated numerically.

Some results are given in figs. 2 and 3. Further results and details will be reported.



DYE LASER INTRACAVITY ABSORPTION FOR ATOMIC
ABSORPTION SPECTROSCOPY

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Dye laser intracavity absorption (ICA) has been shown to be an extremely sensitive means of detecting optical absorption by atoms and molecules. It is particularly advantageous in situations where other forms of absorption spectroscopy, such as resonance fluorescence, photo-acoustic spectroscopy, or the opto-galvanic effect, can not be applied. Such a situation would be in a plasma where background radiation or electrical or acoustic noise interfere with the above methods.

We have been using ICA for several years to study absorption spectra of atoms contained in a microwave discharge and some of the results obtained will be presented. Spectra have been observed in short lived excited states of helium and neon, and in a metastable state of molecular hydrogen all produced in a microwave discharge. Absorption has also been observed in excited states of copper injected into the plasma as well as in the resonance transition of tantalum contained in an atomic beam.

Although the physical phenomena associated with ICA are more complex than those associated with some of the other techniques, it still should be considered whenever it is desired to observe absorption. For example, there are line broadening effects, and the line shape can be complex, but as our work on atomic lithium shows it is possible to achieve good spectral resolution. Data will be presented in which the fine structure of lithium, with a separation of about 0.015 nm, is resolved in an atomic beam. In this case the resolution is limited by the spectrometer.

ICA is a spectroscopic technique that has not received the attention that it deserves. As a means of observing optical absorption, it compliments other techniques, and is often applicable where the others fail or are difficult to apply. It is hoped that this paper will result in other people using this technique.

Elastic Electron Scattering from Atomic Ions:
A Pseudopotential Approach

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ABSTRACT

The integro-differential equations of electron-ion scattering theory are reduced to ordinary differential form by the introduction of a particular class of norm-conserving pseudopotentials, local in exchange and correlation. These potentials are applied to the calculation of elastic scattering phase shifts, bound state eigenenergies, and quantum defects for the Na 2S and He 1P Rydberg series. Quantum defect theory provides both a framework for the calculations and an analytical tool for probing the energy sensitivity of the proposed pseudopotential models. It is found that the uncorrelated potentials reproduce static exchange quality quantum defects accurately throughout the bound spectrum and well across threshold. A simple scaling correction, suggested by analysis of correlation contributions to quantum defects, yields a correlated potential which accounts for the greatest part of core/valence polarization effects. Calculations using the correlated pseudopotentials compare favorably to results derived from the more familiar dipole polarization operator approach.

100% Alignment of Hydrogen Excited States
in Beam-Foil Spectroscopy

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We have measured the relative population production of high n -states in hydrogen following electron capture by fast protons of 50 to 100 keV energy in beam-foil collisions. We observed the photo-emission from high n -states of the Balmer series (up to $n = 15$). The intensity yield $I(n)$ for each principle quantum number follows the law

$$I(n) = I_0 \cdot n^{-(7.0 \pm 0.2)}$$

Adjusting for a lifetime dependence τ proportional to n^{-3} gives a population dependence for the n d states of $n^{-4.0 \pm 0.2}$.

We also measured the linear polarization fraction for emission from the same Balmer lines. We observe the polarization to strongly increase to a maximum of close to 60% for $n = 7, 8$ and 9 and then decrease for higher n . The 60% maximum corresponds to complete alignment of the upper n d state, with all the population being in the $m = 0$ magnetic substate, where the z -axis is taken as the beam axis. The results are shown in the figure below.

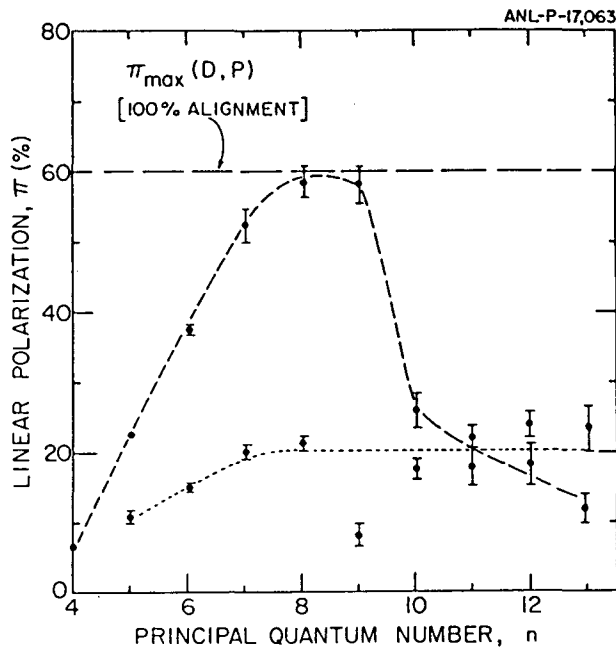


Fig. 1. Linear Polarization fractions for $2p$ - nd transitions in hydrogen following electron pick-up and excitation in a thin carbon foil for 100 keV protons.

The polarization results indicate that the wavefunction of the excited hydrogen leaves the foil as a prolate ellipsoid with major axis along the beam axis. Further experiments show that the proton is not at the center of this wavefunction: we applied a small electric field parallel to the beam axis and measured the field induced quantum beats in the optical decay as a function of distance after the exciter foil. When the field is reversed the quantum beats change in phase by 180° indicating a strong electric dipole moment of the emitting atom. Fig. 2 shows an example of such quantum beats in the $n = 4 - 7$ transition of the Pickering series of HeII.

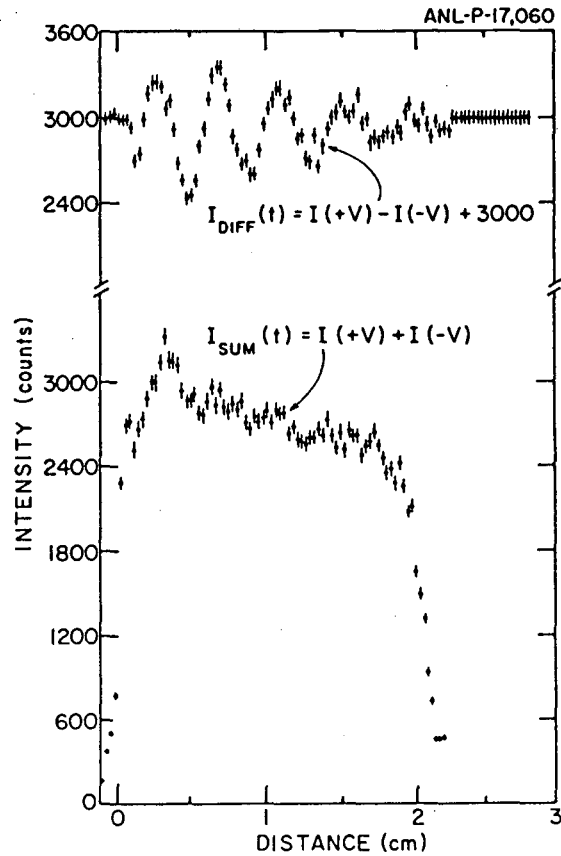


Fig. 2. Decay of the 5411\AA $n = 4 - 7$ transition of HeII in electric fields of ± 200 volts/m.

On the Ground Configuration of the Phosphorus
Sequence from Copper to Molybdenum*

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The energy level structure of the $3s^2 3p^3$ configuration of the phosphorus sequence Mo XXVIII and Zr XXVI ions has been determined from magnetic dipole line wavelengths and emissivities measured in the PLT tokamak discharges. The new measurements have caused some changes in the tentative assignments reported earlier for this sequence,¹ especially for the $^2D_{3/2} \rightarrow ^4S_{3/2}$ transitions. Isoelectronic interpolations together with some experimental confirmations in the Se XX and Ge XVIII spectra now permit a reasonably accurate and complete reconstruction of this configuration from $Z = 42$ to previously established $Z \leq 28$ elements. The measured wavelengths and relative intensities appear to be in substantial agreement with a semi-empirical extrapolation by Kaufman and Sugar.²

*Work supported by U.S. Department of Energy, Contract No. AC02-76-CHO-3073

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Measurements of $1s2s\ ^3S - 1s2p\ ^3P$ Transition Wavelengths
in helium-like Ions in the range $Z = 7$ to $Z = 13$

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We will report measurements of the wavelengths of the $1s2s\ ^3S - 1s2p\ ^3P$ transitions in helium-like Ions of Nitrogen, Oxygen, Fluorine, Neon, Magnesium and Aluminium. Fast beam, recoil-ion and tokamak sources have been used. These measurements will be compared with the results of recent calculations. Measurement and theory now seem to be reliable in the most favourable cases at around the 10 - 20 ppm level for these transitions.

Graphic Analysis of Open-Shell Atom-Chlorine*

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Recent photoionization measurement of autoionization resonances between $3p^4(^3P)$ and $3p^4(^1D)$ ionization limit of chlorine¹ and early data of discrete levels² of atomic chlorine are analyzed based on the graphic method of multichannel quantum defect theory (MQDT)³. One-photon absorption and ionization from ground state, $3p^5(^2P)$, $J=\frac{3}{2}$, leads to 26 channels of configuration $3p^4nl$, $l=s$ or d , and even parity states, 7 channels with $J=\frac{1}{2}$, 10 channels with $J=\frac{3}{2}$ and 9 channels with $J=\frac{5}{2}$. Three sets of Lu-Fano plot corresponding to three different J values are constructed with $3p^4(^3P_2)$ and $3p^4(^1D_2)$ as the first two ionization limits. The basic quantum defect parameters, μ_α and $U_{i\alpha}$ are determined by fitting to the Rydberg levels.

The eigen-phase shift τ_ρ which provides phase shift information in the continuum is obtained from quantum defect plot in the discrete. The channel interaction strength, $\frac{d\tau_\rho}{dv_2}$, is obtained by taking the slope of (τ_ρ, v_2) plot. The dipole moment parameter D_α can be inferred from photoionization data through the relation

$$\frac{df}{dE} = \sum_{\rho} \frac{df(\rho)}{dE} \cong \sum_{\rho} G(D_\alpha, \mu_\alpha, U_{i\alpha}) \frac{d\tau_\rho}{dv_2}$$

Discrete Rydberg levels and autoionization resonances are identified and assigned. New levels are predicted and calculated based on the graphic method. The role of excited state $3s3p^6$, will be discussed. Channel interaction is significant enough to upset the regular fine structure separation, in particular among the d-channels.

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U.V. SPECTROSCOPY OF Al IX - Al XII
FINE STRUCTURE TRANSITIONS AND LIFETIME IN DOUBLY EXCITED Al XI

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The spectra and lifetimes of Al IX - XII have been studied in the wavelength range 15 nm - 61 nm, using the beam foil method with the Orsay - CEV accelerator which gives Al³⁺ ions at 1.15 MeV/amu.

Particular attention is given to the fine structure of the $1s2s2p^4P^{\circ} - 1s2p^2^4P$ multiplet in the doubly excited quartet system of lithium like aluminium. Absolute transition wavelengths have been measured. Results are compared to relativistic predictions. Lifetime has also been measured for the $J = 1/2$ level of $1s2p^2^4P$. A very good agreement is found with recent relativistic calculated transition rates of Chen, Crasemann and Mark.

New transitions in beryllium and boron like aluminium have also been observed.

M.H.CHEN, B.CRASEMANN and H.MARK, Phys.Rev. A 26, 1441 (1982).

A. MCHF-BP STUDY OF THE J-DEPENDENCE OF $3s4p\ ^3P_J$
LIFETIMES IN Mg-LIKE SULPHUR AND CHLORINE

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Accurate lifetimes of atomic levels showing a strong dependence in J have been measured by beam-foil spectroscopy for He-like¹ and Be-like² ions. In these analyses the most prominent cascades are explicitly included through the application of the ANDC method. Similar studies are actually in progress in the Department of Physics, University of Lund (Sweden), for the $3s4p\ ^3P_{0,1,2}$ levels in Mg-like S V and Cl VI³.

Theoretical transition decay rates for these levels and systems will be presented. These data are obtained from multi-configuration Hartree-Fock wavefunctions from which the intermediate coupling eigenvectors are calculated using the Breit-Pauli approximation. The theoretical analysis of the transition probabilities corresponding to the possible decay channels should explain the observed J-dependence of the lifetimes.

¹L. Engström, C. Jupén, B. Denne, S. Huldt, Weng Tai Meng, P. Kaijser, J.O. Ekberg, U. Litzén and I. Martinson, *Physica Scripta* 22, 570(1981)

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³C. Jupén, J.O. Ekberg, S. Bashkin, B. Denne, L. Engström, S. Huldt, A. Trigueiros, U. Litzén, Se. Johansson and I. Martinson, *Atomic Spectroscopy*, University of Lund, Annual report 1981 and private communication.

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Measurement and Analysis of the Atomic Spectrum of Neutral Arsenic^{*}

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The spectrum of neutral arsenic has been remeasured from 1500 Å to 1.2 μ and extended to 4.5 μ. This was done using grating spectrographs at Argonne National Laboratory and Purdue University and the Fourier interferometers at Kitt Peak National Observatory and the Lunar Planetary Laboratory at the University of Arizona. Many new energy levels and classifications have been added to the existing analyses,^{1,2} and a few erroneous levels eliminated. Hyperfine structure splitting constants for many of the levels were determined using interactive software developed by Bruce Pulliam in our laboratory.³ These proved useful as an aid in our analysis. Hartree Fock ab initio calculations were carried out using computer code developed by Robert D. Cowan. The results of these calculations allowed us to assign or change the designations labeling the energy levels. Discrepancies involving the $4s^24p^24d$ and $4s4p^4$ configurations have been resolved. Configuration interaction was found to play an important role, both between pairs of discrete levels as well as between discrete levels and the continuum.

^{*}This work was supported by a grant from the National Science Foundation.

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³B. V. Pulliam, The Decomposition of Hyperfine Structures in Cs II, M.S. Thesis, Purdue University (1979).

ON THE STRUCTURE OF THE TECHNETIUM SPECTRUM

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First the TcI lines were found in the spectra of stars of the late spectral classes [1]. Further investigations [2,3,4] permitted to distinguish the group of stars (about 40), in the spectra of which the lines of TcI were observed (Tc-stars). The possibility to discover the TcII lines (λ 2543 Å, 2610 Å, 2647 Å, 3135 Å, 3195 Å, 3212 Å, 3235 Å) in the solar spectrum was discussed in [5]. Only the line λ 3195 Å, coinciding with one of the weak lines of the Fraunhofer spectrum (FS) of the Sun, was considered. It was noted in [6,7] that while identifying the possible Tc lines in the solar spectrum one has to study the regions of the FS of the Sun, which are both less blended and have comparatively small amount of molecular bands. In these regions the lines λ 4820,74 Å, 4853,59 Å, 5096,28 Å and 6130,81 Å of TcI may be found. The FS spectra of this wavelength region were measured with high resolution and analysed in [8].

For successful study of the astrophysical spectra of Tc the extensive theoretical investigations are of great importance. However, the more or less detail calculations of the Tc spectra are unknown. The TcI spectrum, connected with low configurations, was classified in LS coupling by Moore [9]. The spectra of TcII are known much less.

As the first stage we calculated the energy spectra of the configurations $4d^5 5s^2$, $4d^6 5s$, $4d^6 5p$, $4d^5 5s 5p$, $4d^5 5s 6s$, $4d^6 6s$ and $4d^5 5s 5d$ of TcI. The single-configuration Hartree-Fock numerical wave functions were used as well as an intermediate coupling scheme. The relativistic effects were taken into account as corrections in Pauli approximation. The energy values and the wave functions obtained were used for calculations of the wavelengths and oscillator strengths of some transitions of astrophysical interest. Table illustrates the results obtained. It shows that for better agreement of theoretical oscillator strengths gf_L (length form) with semiempirical gf_S [10] one has to take into account correlation effects. Calculations of such kind as well as the investigations of the spectra of TcII, TcIII and of some elements of the Pd group of astrophysical interest are in progress.

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Transition	J_i	J_f	$\lambda (\text{\AA})$	$g_f L$	$g_f S$
$4d^5 5s^2 6s^-$	2.5	1.5	4238.2	0.08	0.38
$-4d^5 5s(7s)5p^6 P$	2.5	2.5	4262.3	0.14	0.59
	2.5	3.5	4297.1	0.21	0.81
$4d^5 5s^2 6s^-$	2.5	1.5	2608.9	3.5	1.6
$-4d^5 5s(a^5s)5p^6 P$	2.5	2.5	2615.8	5.0	2.5
	2.5	3.5	2614.2	6.1	3.6
$4d^6(a^5D)5s^6 D-$	4.5	4.5	4031.6	3.0	2.5
$-4d^6(a^5D)5p^6 D$	4.5	3.5	3985.0	0.99	0.69
	3.5	4.5	4145.0	0.30	0.18
	3.5	3.5	4095.7	1.2	1.1
	3.5	2.5	4049.1	1.1	0.87
	2.5	3.5	4172.5	0.46	0.28
	2.5	2.5	4124.2	0.35	0.34
	2.5	1.5	4088.7	0.92	0.72
	1.5	2.5	4176.3	0.49	0.33
	1.5	1.5	4136.9	0.021	0.023
	1.5	0.5	4115.1	0.53	0.43
	0.5	1.5	4170.3	0.37	0.27
	0.5	0.5	4145.1	0.12	0.09

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OSCILLATOR STRENGTHS FOR NEUTRAL ATOMIC URANIUM

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By applying the furnace absorption method to the spectrum of neutral atomic uranium, the oscillator strengths for 497 transitions in neutral uranium have been determined in the wavelength interval between 335 nm. and 360 nm. For the strongest transition at 358.48774 nm., the result was $f = 0.044 \pm 0.005$ where the stated uncertainty represents one root mean square variance. This latter result obtained in the pure uranium system may be compared with the absolute oscillator strength, $f = 0.041 \pm 0.003$, derived from opacity measurements in the uranium nitride system. The excellent agreement between these two determinations obtained from two different thermodynamic systems permits the establishing of a single absolute scale for the oscillator strengths in neutral atomic uranium.

ASTRONOMY

NOTES

Invited Speaker

HEAVY ELEMENTS IN COOL STARS

George Wallerstein

University of Washington

Millllions and Millllions of Lines

Robert L. Kurucz

Harvard-Smithsonian Center for Astrophysics

Analysis of solar and stellar spectra and the computation of model atmospheres require data for all lines that contribute significant opacity. In producing opacity tabulations the wavelengths and gf values need be correct only in a statistical sense. In spectrum calculations, however, the wavelengths, gf values, and damping constants must be as accurate as possible in order properly to fit blended features and to determine atmospheric abundances, temperatures, pressures, and velocity fields. My approach to producing line lists is to aim for the highest quality consistent with a large scale treatment, so that even the less successful calculations are quite adequate for statistical opacities. I also adopt whatever good published data are available, although they are usually limited to the strongest lines.

In collaboration with Lucio Rossi of the Istituto Astrofisica Spaziale in Frascati, and with John Dragon and Rodney Whitaker of the Los Alamos National Laboratory, I have computed wavelengths and gf values for over 17,000,000 atomic and molecular lines. Thus far, we have line lists for all the important isotopes of the molecules H_2 , CH, NH, OH, MgH, SiH, CN, C_2 , CO, SiO, and TiO.

In atomic spectroscopy I am now embarked on a program improving and extending the Kurucz-Peytremann calculations of 10 years ago. I determine a Slater integral Hamiltonian by least-squares fitting predicted eigenvalues to observed energies, then use scaled-Thomas-Fermi-Dirac wavefunctions to compute transition integrals, and, finally, use the eigenvectors to transform the complete transition array from LS to the observed coupling, thus producing all possible lines. The observed energies are substituted for the eigenvalues so that the wavelengths are as accurate as possible.

At Los Alamos I have used Robert Cowan's relativistic-Hartree-Fock-with-exchange program to compute starting estimates of the integrals to be used in these calculations. At the present time I have single configuration Slater integrals, configuration interaction integrals, and allowed and forbidden transition integrals for 50 configurations of each of the first 10 ions of the elements up through zinc, and for the first 5 ions of the heavier elements.

I am starting the new calculations with the iron group elements and present results for Fe II as an example.

HYPERFINE STRUCTURE AND THE BROADENING OF SUNSPOT SPECTRAL LINES

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A new atlas of the spectrum of a typical sunspot was completed in 1977 by J. W. Harvey of the Kitt Peak National Observatory. The atlas was made using a polarization analyzer in front of the spectrograph slit. The spectrum shows beautiful patterns, along each absorption line, caused by the Zeeman splitting of the lines in the sunspot magnetic field.

My colleague J. Gethyn Timothy drew my attention to the exceptional width of some of the Zeeman patterns. For one line, that of Mn I at 4070.28A, the broadening appeared to exceed the value predicted by the usual Landé g-factors of the upper and lower energy levels of the line (effective g for the whole line of 3.322 from laboratory measurements, based on the g-values tabulated by C. Corliss and J. Sugar, J. Phys. Chem. Ref. Data 6, 1253, 1977), the observed value being about 3.7. We show that this is an effect of combined Zeeman and hyperfine broadening. Preliminary calculations indicate a combined effective g of 3.71 at 1000 gauss and 3.36 at 3000 gauss. We discuss the need for further hyperfine structure data. We plan further refinement of our calculations.

Branching Ratios and Lifetimes of Uranium and Thorium
Determined from Emission Spectra

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Spectra of uranium and thorium hollow cathode lamps from 250 nm to 5 μm were obtained on the Kitt Peak National Observatory Fourier transform spectrometer. These spectra were corrected for the instrumental response through the use of standard white light sources. The intensities of the lines were measured to an accuracy of $\pm 5\%$ for the stronger lines. Previously measured gf values were used to obtain an excitation temperature (local thermodynamic equilibrium for the excitation was assumed). This allowed gf values for all the assigned lines to be calculated. Branching ratios were determined directly from the measured intensities after suitable corrections were made for the differences in excitation conditions. This allowed lifetimes to be calculated for a large number of levels of uranium and thorium. This is not a precision technique for determining lifetimes, but many approximate lifetimes can be determined rapidly through its use. Comparisons with previously measured lifetimes indicate strengths and weaknesses of this approach.

A New Source for Lifetime Measurements of
Refractory Metal Atoms and their Ions

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ABSTRACT

We report lifetimes of excited states in Nd I, Nd II, U I, and U II using an apparatus recently developed in our laboratory. This device, which uses a Q switched Nd:YAG laser to vaporize the target material, is similar to one described by Bondybey, et al.¹.

We discuss how those operational characteristics of this source, such as vapor pulse shape, neutral density, ion density, and vapor flow velocity, make it suitable for a wide range of spectroscopic applications.

The following table shows a sample of our measured lifetimes compared with others reported in the literature.

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*This work was performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under contract number W-7405-ENG-48.

TABLE

Level (cm ⁻¹)	Lifetime (ns)	
	This work	Others
Nd I 20301	15	10 ± 1.5 ^a
20177	36	35 ± 4 ^a
19770	134	115 ± 11 ^a
16979	600	615 ^c
Nd II 24053	742	
23537	31	
U I 16900	200	205 (+ 10%) ^d
15720	555	
U II 18200	520	520 ^e

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ACCURATE ATOMIC DATA NEEDED IN SOLAR SPECTROSCOPY STUDIES

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A short review will be given of different atomic parameters (transition probabilities, ionization potentials, partition functions, line analysis) which are very important for an improved knowledge of the solar photosphere. The role of a very accurate knowledge of these parameters on the determination of the abundances of the elements in the sun and on the determination of the physical structure of the solar photosphere will be stressed.

A summary of new solar abundance results recently obtained in collaboration with different groups in Berlin, Melbourne and Caltech, using accurate transition probabilities, will be presented.

Ionization Potential of Neutral Iron, Fe I,
by Laser Spectroscopy†

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ABSTRACT

We have determined the ionization potential of Fe I by three step laser excitation to produce an autoionizing Rydberg series with high n^* (~ 28 to ~ 52) that converges to the second ionization limit 384.77 cm^{-1} above the ionization potential of neutral Fe. The method used has been described in detail in the literature¹. The three steps used were laser 1 at 3824.444 \AA ($0 - 26140.19 \text{ cm}^{-1}$, $J = 4$ to 3), laser 2 at 5283.621 \AA ($26140.18 - 45061.33 \text{ cm}^{-1}$, $J = 3$ to 3) and laser 3 scanned from 5310 to 5240 \AA to produce the autoionizing series. The limit $64122(2) \text{ cm}^{-1}$ found for this series yields an ionization limit of $63737(2) \text{ cm}^{-1}$ [$7.9024(2) \text{ ev}$] for Fe I. This ionization limit is considerably more accurate than current values, $63700(80) \text{ cm}^{-1}$, 63400 and $63480(500) \text{ cm}^{-1}$ available in the literature.^{2,3} We intend to observe other series and attempt to further reduce the error limit on the ionization potential. This precise value should be useful to astrophysicists, plasma physicists and theorists.

† This work was performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under contract number W-7405-ENG-48.

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