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SEMIEMPIRICAL STUDIES OF ATOMIC STRUCTURE

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I. SCOPE OF INVESTIGATIONS

The energy level structure, transition probabilities, and general spectroscopic properties of highly-ionized many-electron systems are studied through the combined use of sensitive semiempirical data systematizations, selected precision experimental measurements, and specialized theoretical computations. Measurements are made primarily through the use of fast ion beam excitation methods, which are combined with available data from laser and tokamak produced plasmas, astrophysical sources, and conventional light sources. The experimental studies are strengthened through large scale *ab initio* calculations. Large blocks of data are predictively systematized and parametrized along isoelectronic, homologous, isoionic, Rydberg, and yrast series, to provide a comprehensive and reliable data base.

II. SIGNIFICANT RESULTS

During the period from 1 March 1992 - 15 December 1992, work done as part of this project has resulted in eleven papers published or submitted for publication [1-11]. This has been done using experimental fast-ion-beam measurements, theoretical calculations, and semiempirical systematizations of spectroscopic data. A few typical examples will be described below.

Lifetime measurements in the neon isoelectronic sequence. Because of the strong radiative decay of the $2p^6-2p^53s$ transitions in the Ne isoelectronic sequence, it is possible to create a population inversion between the $2p^53s$ and $2p^53p$ levels which can produce XUV laser amplification action. Modeling studies have demonstrated that amplification is optimal near $Z=36$, leading to applications to Se and Y plasmas. The lifetimes of these levels are too short for time-of-flight measurements at $Z=36$, but we have developed methods that permit reliable semiempirical extrapolation if precise results at lower Z are available. We have performed precision measurements of the $2p^6 - 2p^53s - 2p^53p$ transitions in S VII and Cl VIII. These studies were made possible by the existence of a uniquely designed beam-foil chamber at the University of Lund which views a very short segment of beam with a grazing incidence monochromator, permitting the precision measurement of lifetimes as short as few ps for wavelengths well below 100 Å. These measurements yielded lifetimes accurate to 3-4%, as compared to earlier measurements which had uncertainties $\geq 25\%$. In addition to the curve fits, it was also possible to perform ANDC correlated decay analyses with the primary cascade channel $2p^53s-2p^53p$ (the laser transition). We have applied a semiempirical technique which determines an effective singlet-triplet mixing angle ϑ from spectroscopic energy level data, and divides the line strength of the resonance line by $\cos^2\vartheta$ and that of the intercombination line by $\sin^2\vartheta$. In earlier studies of a variety of isoelectronic sequences, this plot has been found to be empirically linear, and if extrapolated to Se ($Z=34$) it implies lifetimes for the resonance and intercombination lines of 0.13 and 0.55 ps. While this approach is somewhat speculative, existing *ab initio* calculations vary by factors of 2, and a semiempirical approach that is extrapolatively reliable to the 3-4% levels of accuracy provided by our measurements is valuable for modeling purposes.

Multiplexed decay curve measurements of Li-like Si XII. We have utilized position sensitive detection of VUV emission from excited fast silicon ions to make precision measurements of the J dependence of the lifetimes of the 2s-2p multiplet in Li-like Si XII. The experiment was carried out at the Notre Dame Tandem Accelerator in collaboration with A.E. Livingston of Notre Dame and H.G. Berry of ANL. The 42 MeV foil-excited Si beam was viewed with a 1 m normal incidence monochromator, using a detector consisting of a 1 inch wide windowless channeled electron multiplier array in the chevron configuration, coupled with a resistive anode position sensor. The position decoding of the photon induced pulses was obtained by comparison of the divided pulse charges appearing at the two ends of the anode. The two strongest lines are the 2s-2p fine structure resonance transitions (in 2nd order), and the other features arise from the Si XII n=5-6 and Si XI n=6-7 Rydberg transition complexes. This multiplexed registration provides a more precise determination of the relative lifetimes through the cancellation of the small systematic effects (beam fluctuations, degradation of foil quality, etc) that limit the accuracy of separately measured decay curves. When reduced to eliminate λ^3 dependences, the measured line strength ratio was $S(1/2-3/2):S(1/2-1/2)=1.979(44)$, which can be compared with *ab initio* calculations of 2.007 (MBPT) and 2.005 (MCDF), and a semiempirical calculation of 2.007 (CAHS). This type of multiplexed decay curve measurement offers new possibilities for improved accuracy in lifetime measurement. As one example, it could permit sensitive measurements of the relative lifetimes of fine structure components where CI or IC selectively couples a particular J level to produce an additional intercombination or autoionization channel. It also makes possible the real-time application of the ANDC correlated analysis of cascade repopulation for a system if the primary and cascade transitions are within the same wavelength range.

Isoelectronic specification of intershell resonance and intercombination decay rates using measured transition probabilities and spectroscopically determined singlet-triplet mixing amplitudes. Methods recently developed to specify alkaline-earthlike $\Delta n=0$ intrashell transitions of the form $ns^2 - nsnp$ were extended to intershell transitions $2s^2 - 2s3p$ levels in the Be isoelectronic sequence. These transitions provided a stringent test of these methods, since they are affected by plunging configuration interaction, transition integral cancellations, and multiple exit channels that were not present in the intrashell transitions. Experimental measurements of the intercombination transition probabilities were accessible by virtue differential decay curve measurements that exploit the J dependence of the exit channels of the triplet levels. Using our own measurements for intercombination rates in N IV, O V, F VI, and Ne VII, a joint linearizing formulation was obtained that also predicts the lifetime of the resonance transition. The homologous counterpart given by the $3s^2 - 3s4p$ levels in the Mg sequence was also studied using existing measurements for S V and Cl VI. Here the $3p3d$ configuration introduced significant plunging configuration interaction and additional intercombination channels. This produces heavy CI effects in S V which are not present in Cl VI. It was possible to characterize the CI as indirect rather than direct because the singlet-triplet mixing amplitudes obtained from the spectroscopic data removed the isoelectronic irregularities from the reduced transition probability data.

III. BIBLIOGRAPHY OF PUBLICATIONS PRODUCED ON THIS PROJECT

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