DISCREPANCIES BETWEEN THEORETICAL AND EXPERIMENTAL ATOMIC OSCILLATOR STRENGTHS OF THE SODIUM ISOELECTRONIC SEQUENCE RESONANCE TRANSITION

R.J.S. CROSSLEY* and L.J. CURTIS**
Research Institute for Physics, S-10405 Stockholm 50, Sweden

and

Charlotte FROESE FISCHER
Department of Computer Science, The Pennsylvania State University, University Park, Pennsylvania 16802, U.S.A.

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Discrepancies between theoretical and experimental estimates of the oscillator strengths of the sodium isoelectronic sequence resonance transition are considered in the light of recent multi-configuration Hartree-Fock results. Possible experimental difficulties in the cascading analysis arising from a peculiar pattern of excited-state lifetimes are examined using computer simulations of decay curves.

The 3s–3p resonance transition of sodium-like ions has not been expected to pose theoretical problems. Nevertheless recent experimental work by the beam-foil technique has led to measurements of oscillator strengths significantly lower than theoretical values. Calculations by one of us appear to exclude the possibility that these discrepancies are due to shortcomings on the theoretical side. Since the experimental situation is complicated by a peculiar pattern of lifetimes of excited states for the higher isoelectronic ions of the alkali sequences, we have investigated the effects of cascading on the extraction of the 3p lifetime from its decay curve.

Fig. 1 shows the oscillator strength data, plotted against inverse nuclear charge Z^{-1}, for $Z < 30$. The solid curves I–V represent calculations with the dipole-length matrix element and experimental energies. Experimental data for the ions are as referenced by Laughlin et al. [1] with two more recent values: PV, $f = 0.60$ [2] ; Ar VIII, $f = 0.45$ [3] ; and one omission [4] . (The S VI point of Berry et al. (1970) was attributed to a cascade component by the authors in a note added in proof, a fact subsequently verified by Andersen et al. [4] , and should not be cited in isoelectronic comparisons.) Beam-foil results are shown by circles, and other experimental methods are indicated by crosses. The Na I value is from the NBS tables [5] .

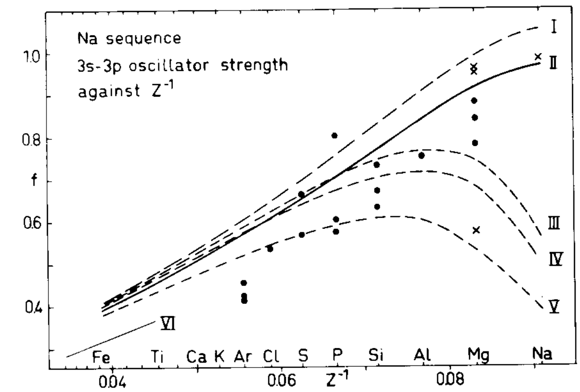

Fig. 1. For explanation see text.

The trend of beam-foil results, which are generally expected to be accurate to about 10% [6] , clearly lies well below the Hartree–Fock results [7] (curve I), the discrepancies ranging from about 15% for the

* Permanent address: Department of Mathematics, University of York, York Y01 5DD, U.K.
** Permanent address: Department of Physics and Astronomy, University of Toledo, Toledo, Ohio 43606, U.S.A.

lower ions to 28% for Ar VIII, and is inconsistent with the non-relativistic high-Z behaviour indicated by the asymptotic tangent VI [1]. Core polarisation has been suggested as an explanation [8] despite calculations which show this effect to be only about 4% [e.g. 9]. This small figure is confirmed by the multi-configuration Hartree–Fock calculations of Froese Fischer [10] (curve II) which allow for pair-correlation and achieve reductions from the Hartree–Fock results ranging from 8% (Na I) and 6% (Ar VIII) to only 4% (Fe XVI). A much larger polarisation correction has been claimed by Laughlin et al. [1] using the exact Z-expansion method (curve V; compare the Hartree–Fock Z-expansion results curve IV [11]), but this is clearly a figment of these calculations being cut off at first order; calculation to second order in the Hartree–Fock scheme [12] (curve III) gives much better results. Relativistic effects are negligible for $Z < 30$ (and in fact increase the oscillator strength [8]). We therefore conclude that curve II is correct to within 5% and substantial discrepancies in the higher ions remain to be explained on the experimental side.

Fig. 2 compares the pattern of lifetimes for Na I with those of Ar VIII (multiplied by $(Z-10)^4$ so that the higher lying level lifetimes will approach hydrogenic values [13] for both). The differences are striking. In Na I the 3p lifetime is shorter than any of its cascades, while for Ar VIII the 3p lifetime is an order of magnitude longer than its close lying cascades, and the strong unbranched "yrast" ($l = n - 1$) cascade lifetimes increase outwardly to very high values. The origin of these effects can be traced to the core penetration of the 3s and 3p levels in the Na I sequence, which increases with increasing ionization [14]. Thus it might be suspected that this decay curve will contain unusually strong cascades effects which could complicate the experimental analysis. We have therefore studied this system using theoretical meanlives and branching ratios with model populations.

Fig. 3 shows a computer simulated set of decay curves for the logarithm of the detected intensity for this sequence, with the time coordinate in units of the 3p meanlife. The simulation includes 18 indirect yrast cascades and 5 direct Rydberg cascades initially populated in proportion to $(n^*)^{-3}$, and is convoluted with an instrumental resolution of 0.5 ns. A number of other population models [15] were also tested but produced qualitatively similar decay curves. The results are quite surprising and indicate that, despite these very strong cascade effects, the 3p meanlife (indicated by the dashed line) should be extractable for all of these charge states. The curves also suggest a possible pitfall arising from the long lived cascades, which could easily be overlooked for the higher charge

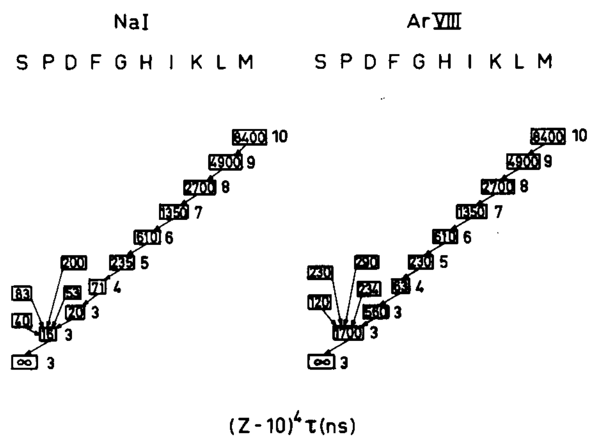

Fig. 2. Level schemes for (a) Na I and (b) Ar VIII. The boxed numbers are the individual level lifetimes.

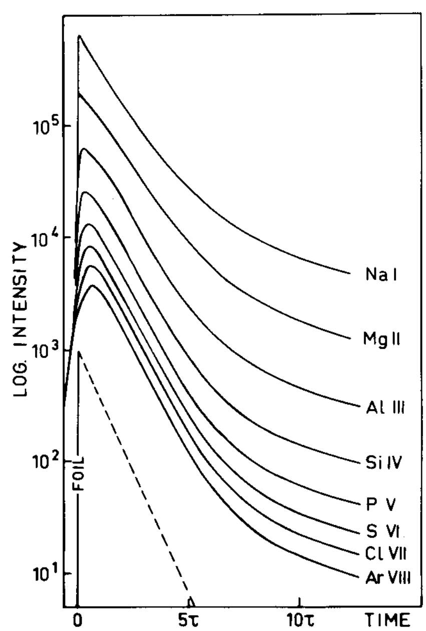

Fig. 3. Computer simulated decay curves for the 3s–3p transition including 19 yrast and 4 Rydberg cascades and an instrumental resolution of 0.5 ns.

states if the decay curves were followed for only a few 3p meanlines or were concealed by statistical uncertainties. Several of the experimental results cited report no long lived cascading. Detailed calculations are in progress, using meanlives and branching ratios obtained from a numerical Coulomb approximation program [16] to include cascade effects from any more levels, which it is hoped will permit a quantitative assessment of this loss of accuracy.

We conclude that theoretical estimates for the higher charge states of this sequence are accurate to within ± 5%; similar results should be extractable from experimental decay curves provided these can be followed for at least ten 3p meanlines with good statistical accuracy.

References

[1] C. Laughlin, M.N. Lewis and Z.J. Horák, Astrophys. J. 197 (1975) 799.

[2] A.E. Livingston, J.A. Kernahan, D.J.G. Irwin and E.H. Pinnington, Phys. Scripta 12 (1975) 223.

[3] A.E. Livingston, Thesis, University of Alberta (1974).

[4] T. Andersen, A. Kirkegård Nielsen and G. Sørensen, Nucl. Instr. Meth. 110 (1973) 143.

[5] W.L. Wiese, M.W. Smith and B.M. Miles, Atomic Transitions Probabilities, vol. II (NBS Washington D.C. 1969).

[6] E.H. Pinnington, A.E. Livingston and J.A. Kernahan, Phys. Rev. A9 (1974) 1004.

[7] E. Biémont, J.Q.S.R.T. 15 (1975) 531.

[8] W.L. Wiese and S.M. Younger, in Proc. Fourth Intern. Beam-Foil Spectroscopy Conf. (Plenum Press, New York 1976).

[9] J.H. Black, J.C. Weisheit and E. Laviana, Astrophys. J. 177 (1972) 567.

[10] C. Froese Fischer, Technical Report No. 174, Computer Science Department, Pennsylvania State University (1975).

[11] R.J.S. Crossley and A. Dalgarno. Proc. Roy. Soc. A286 (1965) 510.

[12] C. Froese, Astrophys. J. 141 (1965) 1206.

[13] W.L. Wiese, M.W. Smith and B.M. Glennon, Atomic Transition Probabilities, vol. I (NBS, Washington, D.C. 1966).

[14] B. Edlén, Handbuch der Physik 27 (1964) 80.

[15] R.M. Schectman, Phys. Rev. A12 (1975) 1717.

[16] A. Lindgård and S.E. Nielsen, J. Phys. B8 (1975) 1183.