SECTION II

EXCITATION AND IONIZATION: THEORY AND EXPERIMENTS

Chairman:

J. KISTEMAKER

THEORETICAL STUDIES ON TRANSITION WAVELENGTHS AND TRANSITION PROBABILITIES

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A discussion is presented of some theoretical methods for predicting atomic transition wavelengths and transition probabilities that are especially useful for highly stripped ions. Particular attention is given to procedures involving model potentials and pseudopotentials and to procedures involving expansions in inverse powers of the nuclear charge. The importance of relativistic effects is assessed. The results of some recent calculations are compared to experimental data. Theoretical studies of molecular absorption and emission are briefly summarized.

DISCUSSION

A.H. Gabriel: For autoionzation rate calculations, what is the status of close coupling methods?

A. Dalgarno: Close-coupling calculations of the conventional kind appear to be practicable only for the low-lying resonances of simple systems.

A.H. Gabriel: For non-autoionizing states like $2p3p^3P$, how far up the isoelectronic sequence must one go before spin-orbit interaction enables autoionization to proceed?

A. Dalgarno: Explicit calculations are needed to answer your question. I might guess that autoionization would not be competitive for nuclear charges less than 10.

W.R.S. Garton: Regarding Dr Gabriel's enquiry on the possibility of spin-orbit interaction promoting autoionization, even when electrostatic configuration – mixing is absent, we should note that the former yield an autoionization lifetime longer by about $\alpha^4 \sim 10^8$. Thus, if we regard 10^{-13} s as a typical autoionization decay time for the electrostatic mixing, we expect 10^{-5} s in the case of spin-orbit and this would yield 'unbroadened' lines, in ordinary terms.

R.W. Nicholls: I wonder if you would care to make any comparable comments on the state of molecular theory?

A. Dalgarno: There appears at present to be no way of predicting molecular transition probabilities with any useful reliability except by extremely laborious time-consuming variational calculations.

R.W. Nicholls: Does that include the *ab initio* calculations of Clemente, Maclean Roothaan and others?

A. Dalgarno: Yes.

J. Kistemaker: How do the 1^1S–2^3P transition rates, measured recently in Ar XVII at Berkeley, compare with your calculations?

A. Dalgarno: Theory and measurement agree to within the experimental error.

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