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THEORETICAL STUDIES OF ELECTRONIC TRANSITION LASERS. (U)
1979 M KRAUSS, W J STEVENS

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$X^2\Sigma^+ - A^2\Pi$ transition, shown in Fig. 2, as a function of the transition energy.

A preliminary analysis of the energetics of the excimer states for the rare gas halides has also been made. Weak radiative transitions play several roles in this case. They provide diagnostics or can be used to photodissociate or pump higher states. In addition, the presence of the B→A radiative transition complicates the analysis of the kinetic data with regard to both the relative B and C energies and the quenching of these states.

Four notes have been published or submitted to date. Titles and abstracts are listed below. We greatly benefited from the assistance of guest workers from the Chemistry Department of SUNY, Binghamton, M. E. Rosenkrantz and D. D. Konowalow. A paper on the "The Electronic Structure and Spectroscopy of the X,A, and B States of HgCl" is in preparation.

The abstracts provide a summary of our conclusions. The self-absorption calculations on HgCl are completed. Questions still remain concerning the ordering of the B and C states in the rare-gas halides. During FY80 we will extend our calculations to the rare gas halide triatomic systems in order to estimate the role of these species in the kinetics and radiative properties of high pressure rare-gas halide laser mixtures. Photodissociation calculations of the X→A transitions in the diatomic rare gas-halide molecules will also be used to probe problems in the temperature dependence of the efficiency for systems with significantly bound X states.

II. Titles and Abstracts

1. Photodissociation of HgCl
P. S. Julienne, D. D. Konowalow, M. Krauss, M. E. Rosenkrantz,
W. J. Stevens
To be published Applied Physics Letters.

Transition moments and energies have been calculated for the X-A, bound to continuum, transition in HgCl. The photodissociation cross section at the peak is $1.2 \times 10^{-18} \text{ cm}^2$ at 600K. The laser energy for the B-X transition is close to the peak energy and a significant absorption will result from a buildup in the concentration of X state HgCl in the course of exciting the laser media. The absorption is suggested as an explanation for the low extraction efficiencies observed for HgCl lasers.

2. Dipole Polarizabilities of Zn, Cd, and Hg (1S).
D. D. Konowalow, M. E. Rosenkrantz, W. J. Stevens, and M. Krauss
Chem. Phys. Lett. 64, 317 (1979).

Effective core potentials (ECP) are used in a calculation of the dipole polarizability of the ground states of the Zn, Cd, and Hg atoms. The trend in the magnitude of the polarizability as a function of increasing Z of the recommended values is reproduced in the calculated polarizabilities using relativistic ECP. Polarizabilities obtained with non-relativistic ECP do not reflect the observed trend and are much too large in magnitude.

Compact atomic bases, useful for molecular calculations, are obtained by optimization of the function exponents with respect to both the energy and polarizability.

3. Dipole Polarizabilities of the Group II b-Atoms Obtained From Compact Variational Trial Functions.
M. E. Rosenkrantz, W. J. Stevens, M. Krauss, and D. D. Konowalow
To be published J. Chem. Phys.

In order to optimize basis sets for future molecular calculations, the energies and dipole polarizabilities of 1S , 3P , and 1P states of Zn, Cd, and Hg have been determined from Hartree-Fock (HF) and multi-configuration calculations. These utilize either empirically fitted pseudopotentials or ab initio effective core potentials (ECP). Our calculated polarizabilities for ground state atoms agree within 10% with recommended values so long as either the empirical pseudopotentials or the ECP based on relativistic HF calculations are used. Our calculations agree with the measured anisotropy of the polarizability of 3P_1 Hg, but disagree with measured values of the 3P_2 state anisotropy. Our calculated 3P_2 anisotropy is consistent with both the measured and calculated 3P_1 Hg anisotropy; the measured 3P_2 values are not. We find calculations based on non-relativistic ECP to give incorrect polarizabilities.

4. Role of the III $1/2$ - II $1/2$ Transition in Rare Gas Halide Kinetics.
P. S. Julienne and M. Krauss
Applied Physics Letters 35, 55 (1979).

Rare gas halide spectra have previously been analyzed in terms of the strong III $1/2$ - I $1/2$ lasing transition and the weaker II $3/2$ - I $3/2$ broad continuum. However, the III $1/2$ - II $1/2$ transition is also a broad continuum that strongly overlaps the II $3/2$ - I $3/2$ transition and has an Einstein coefficient of a similar magnitude. The existence of this transition requires a reinterpretation of previous kinetic data on ArF, KrF, XeF. Simultaneous energy extraction from both the III $1/2$ and II $3/2$ states should be possible for lasing in the broad continuum.



