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Applied Quantum Chemistry

Advanced Laser Development

MASTER

Final Progress Report
for the Period

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1 October 1978 - 30 September 1979

M. Krauss, W. J. Stevens, P. S. Julienne, F. H. Mies

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U. S. Department of Energy
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Application of Quantum Chemistry to Laser Chemistry

I. Introduction

Efficient extraction methods can not be identified if the spectroscopic behavior of the active laser media is not well understood both in terms of the assignment and intensity of the transition. This is particularly true of excimer, metastable, or collision-induced laser candidate systems. Theoretical calculations have been a primary source of information for the rare gas halide spectroscopy but a serious difference between experimental and theoretical interpretations needs to be resolved. For the group IIb homonuclear systems experimental information on gain and assignments has been very hard to obtain. Assessment of Raman methods of extraction require theoretical calculation as well as a new analysis of the spectroscopy of continuum processes with degenerate asymptotes.

The use of rare gas halide pumped Raman amplifiers is obviously limited by absorption processes. Collision-induced absorption for either pump or Stokes radiation will severely limit the efficiency. The calculation of the collision-induced absorption require a knowledge of the energy curves of the ground and excited states and the induced transition moment as a function of the internuclear distance. Such calculations have been carried out for lead interacting with rare gases and concluded that absorption is not significant for XeCl pump radiation.

The calculations were made possible by significant improvements in the electronic structure codes by implementing pseudopotential capability

for both non-relativistic and high Z , relativistic atoms. Calculations on the rare gas halides were also improved to show that the B state is lower than the C for both XeF and XeCl. All the minor transition moments were also calculated to provide a basis for photodissociation and pumping analyses.

The various problems analyzed this year will be briefly summarized below. The summaries give our conclusions on these problems. The summaries are divided into three categories. First, the theoretical analyses of Raman processes in intense fields are described. Second, the electronic structure calculations are presented with a brief description of pseudopotential code development. Third, the analysis of absorption processes, both collision-induced and photoionization, and energy transfer processes is presented.

II. Raman Processes in Intense Fields

a. Resonance Fluorescence and Raman Line Shapes Produced by Monochromatic Laser Fields: Effects of Branching Ratio and Homogeneous Broadening.

F. H. Mies

The Heitler-Ma damping theory is developed for a two level system in which the excited state is homogeneously, and irreversibly coupled to various continuum states with a total decay rate $1/\tau$. We give particular consideration to the channel consisting of a third, discrete, atomic level and a continuum of emitted photons, which simply corresponds to a spontaneous resonant Raman process. The theory applies to either a narrow, pulsed, laser beam, or injection of target atoms or molecules into a c.w. field.

In this paper we examined the $t = \infty$ spectra as a function of a field strength, detuning from resonance, and especially as a function of the upper state broadening, characterized by the branching ratio $f_A = \tau/\tau_A$, where τ_A is the natural resonance fluorescence lifetime. For strong fields we obtain the usual resonance fluorescence spectrum centered at the incident, pumping frequency, with two symmetric side bands displaced by the Rabi frequency. If $f_A \rightarrow 0$ the spectrum approaches the "one-photon" limit, with the side bands equal to $1/2$ the central peak. In this limit the target predominantly decays into the Raman, or other irreversible channels, and only a single cascade contributes to the extremely weak resonance spectrum. At the opposite extreme, $f_A \rightarrow 1$, the spectrum exhibits the infinite cascade properties obtained by Mollow,

etc., with the side bands broadened, with a height equal to $1/3$ the central peak. In this theory we obtain a more complete interpretation of the "elastically scattered delta function" which is an artifact of the infinite lifetime of the atom in the usual two level theories. In both limits we obtain a continuum (Raman) spectrum which is unchanged, and is simply a function of the total width $\hbar/\tau$ of the excited state.

b. Kinetics and Spectroscopy of Near-Resonant
Optical Pumping in Strong Fields.

F. H. Mies and Y. Ben-Aryeh

Optical pumping occurs whenever the upper molecular state in a resonant absorption process can undergo irreversible decay into a continuum state. We consider an extreme level of optical pumping where intense pulsed laser beams can deliver coherent packets of photons in sufficient numbers, and in times sufficiently short compared to equilibrium relaxation times, that the photons may be considered a principal reagent in a photochemical reaction and entire populations of molecules or atoms are transformed from one side to another by inelastic resonant photon scattering. We examine the transient behavior for the process, the final distribution (spectroscopy) of the continuum states, and some aspects of the saturation and non-linear effects caused by the intense fields.

We especially want to examine, and exploit the role of dressed states in a proper description of the strong field effects. We present an exact solution of the Heitler-Ma damping theory for the process which is valid over the entire range of Rabi frequencies and incorporates the saturation effects without introducing the dressed states explicitly. The results allow for a better understanding of the restrictions, and virtues of the limiting cases and provides a well-defined model which can be compared to the approximate theories.

c. Optical Pumping of Excimer Storage Lasers:
Expectations and Limitations.

F. H. Mies

A theoretical model for optical pumping in strong fields is developed using dressed-states to describe near-resonant interaction with the pumping field. Explicit expressions are obtained for the gain experienced by an excimer extraction pulse which couples to the upper states in the absorption process. Estimates are made of critical parameters which influence the extraction time and the efficient extraction of energy stored in the reservoir of metastable states. An interesting result is obtained in the limit of high pumping field strengths E_0 . The high density of accessible molecular states systematically prevents a complete saturation of the pumping rate which passes from an E_0^2 to an E_0 dependence in high field limit.

d. A Scattering Theory of Diatomic Molecules: General Formalism Using the Channel State Representation

F. H. Mies

We present a unified theory of diatomic molecules which reconciles bound state spectroscopy and atomic scattering theory. The total wavefunction is expanded in a complete set of atomic channel states and careful consideration is given to the constraints imposed by proper asymptotic boundary conditions. Below the first dissociation limit all channels are closed and well-behaved solutions are obtained only at specific eigenvalues with total energies which correspond to the usual electronic-rotational-vibrational states of the molecule. Above this limit we have the scattering wavefunctions for the atomic fragments. Imbedded in the open-channel continua are closed-channel resonance states which are identical to the predissociating states of diatomic spectroscopy.

The expansion in channel states is entirely equivalent to an expansion in Hund's case (e) electronic-rotational states. The scattering formalism places strong constraints on the asymptotic properties of the radial, i.e., vibrational, functions which are represented in terms of the K and S matrices of scattering theory. Careful consideration is given to the properties of closed-channels which represent the bound states of conventional spectroscopy. The normalization of the total wavefunctions is derived and related to the asymptotic boundary conditions both for continuum and bound states.

e. A Scattering Theory of Diatomic Molecules:
Expansion in Adiabatic Electronic-Rotational States.

F. H. Mies

An exact theory of diatomic molecules must be consistent with atomic scattering theory. In general scattering wavefunctions can not be factored into electronic-rotational and radial terms. Yet the starting point of most diatomic analysis is the Born-Oppenheimer Approximation (BOA) which factors the total molecule wavefunction into an electronic-rotational function and a radial or vibrational function which yields the Franck-Condon principle. This is a severe approximation which is at best valid for small amplitude vibrations, may be expected to fail near dissociation limits, and is completely invalid in the dissociation continuum.

In the preceding paper we presented a complete theory of the total molecular wavefunction in terms of atomic channel states which gives a unified description of diatomic states throughout the entire spectrum.

In this paper we perform an orthogonal transformation on the channel states and expand the total wavefunction in a complete set of adiabatic electronic-rotational states. These states are implicit, analytical functions of the interatomic coordinate, R , and progressively change from one Hund's electronic-rotational coupling case to another as R is varied. At infinity they approach pure Hund's case (e) which are, in fact, the proper atomic channel states we require to describe the scattering boundary conditions. At finite R they transform to the usual Hund's cases appropriate to bound-state spectroscopy.

The coupled equations are developed using the adiabatic representation, and the exact solutions are expressed in terms of the regular, and irregular solutions of the adiabatic interaction potentials. Deviations from the BOA can be expressed in terms of an R-dependent reactance matrix, and an R-dependent normalization matrix which can be obtained from solutions of the usual closed-coupled equations of atomic scattering theory.

III. Electronic Structure: Assignments and Gain Cross Section.

a. Pseudopotential Code Development.

W. J. Stevens

During the term of this contract an extensive set of computer codes has been developed for atomic, diatomic, and polyatomic electronic structure calculations based on the effective core potential (ECP) approximation. In this approximation, the chemically unimportant atomic core electrons are replaced by a local potential which simulates the energetic interaction between the valence electrons and the core. This approximation essentially opens the entire periodic table to investigation within the framework of standard multiconfiguration self-consistent-field (MCSCF) and configuration interaction (CI) techniques.

Codes have been implemented to derive ECP from either experimental spectroscopic data or ab initio atomic structure calculations. The empirical potentials are best suited for alkali and alkaline earth species, and are based on fitting the observed spectroscopic terms for a single electron outside the core. Core polarization effects can be added, and are essential for the heavier Group IA and Group IIA elements. The ab initio based potentials are derived from numerical Hartree-Fock wavefunctions by the method outlined by Kahn and coworkers. Either non-relativistic or relativistic Hartree-Fock wavefunctions can be used, with the latter being averaged to yield L-dependent potentials from the J-dependent Hartree-Fock solutions.

The electronic structure programs into which these potentials have

been introduced include an extremely efficient atomic self-consistent-field (SCF) code which has the capability of automatic exponent optimization for the development of basis sets of varying complexity for use in subsequent molecular calculations. A unique feature of this code is the possibility of wavefunction optimization in the presence of an applied electric field, which allows us to produce polarization basis sets and first order wavefunctions. In addition to the atomic code, we have interfaced the ECP programs with the IBM ALCHEMY molecular structure codes. These codes are among the most sophisticated in the world for molecular SCF, MCSCF, CI, and properties calculations.

This powerful program library has been applied to a variety of laser-related calculations including the Group II metal dimers, the rare-gas halides, the Group II halides, and the Group II-rare gas dimers.

b. Oscillatory Excimer Emission: An Analytic Model

F. H. Mies and P. S. Julienne

An analytic quantum mechanical model is given for the line shape of the continuum emission from a model harmonic oscillator excimer state to a flat lower state. The model permits a qualitative characterization of the excimer emission profile for more realistic potentials and permits an estimate of bounds on excimer gain cross sections. The model is best on the red wavelength side of the spectrum, and it gives a good account of the McLennan bands of I_2 . An Appendix discusses semiclassical approximations to the spectrum in a unified way. The stationary phase approximation is shown to lead to an expression very similar to the exact quantum result, and a new nondivergent approximation is derived from the red limit of the spectrum.

c. Energy Curves and Transition Moments for XeF and XeCl.

W. J. Stevens and M. Krauss

First-order configuration interaction calculations have been carried out on the ground and low-lying excited states for XeF and XeCl using effective core potentials (ECP) to replace the core electrons. Since these calculations were intended to verify the energy ordering of the B and C states of these molecules, very careful basis set optimizations were done in order to accurately describe the excited charge transfer states. Although the B and C states are found to be several tenths of an eV deeper and, consequently, the predicted emission frequencies are closer to experimental values, the present results support the energy ordering calculated earlier by Hay and Dunning (J. Chem. Phys. 69, 220 (1978)).

The improved basis yields binding for the $X^2\Sigma$ covalent state in both XeF and XeCl. Damped dispersion interactions have been calculated for both systems for the dipole-dipole and dipole-quadrupole interactions. Including spin-orbit interactions in semi-empirical fashion permits a fairly complete description of binding in these molecules.

Transition moments have been obtained for all transitions for $\Delta\Omega=0, \pm 1$. The weak $\Delta\Omega=\pm 1$ transitions are usually ignored but they provide a means of probing or pumping the excited states. The weaker $\Delta\Omega=0$ transitions such as the B $\rightarrow$ A will also play a role in the analysis of the broad-band emissions even for the fluorides and chlorides and must be known accurately.

d. Cd_2^* as a 470nm Absorber.

W. J. Stevens

Multiconfiguration self-consistent-field calculations have been carried out on all of the valence states, low-lying rydberg states, and charge-transfer states of Cd_2 . Like the other Group IIb dimers studied thus far, the lowest excimer level was found to be a $^3\Pi_g$ metastable state that acts as a reservoir for molecular excitation energy. Strong absorptions between this reservoir state and a bound $^3\Pi_u$ charge-transfer state and a bound $^3\Pi_u$ charge-transfer state are predicted in the vicinity of 470nm. These absorptions essentially rule out Cd_2^* as an excimer laser candidate, and may also have serious implications for proposed CdHg^* lasers.

e. Spectroscopy of Lithium and Sodium Dimers.

D. D. Konowalow and P. S. Julienne

The triplet manifold of states in the low-Z alkali dimers are essentially unknown spectroscopically. However, recent quantum mechanical calculations for Li_2 and Na_2 provided accurate potential curves for the low lying states. The $^3\Sigma_g^+ - ^3\Sigma_u^+$ system offers the possibility of an excimer laser or tunable optical converter in the infrared.

We have calculated the dipole transition matrix elements for the $^3\Sigma_g^+ - ^3\Sigma_u^+$ and $^3\Sigma_g^+ - ^3\Pi_u$ transitions. The calculated $^3\Sigma_g^+$ radiative lifetimes decrease slowly with increasing vibrational quantum number, ranging from 62 nsec for $v'=0$ to 40 nsec for $v'=10$. The decay rate for $^3\Sigma_g^+ - ^3\Pi_u$ is much weaker than that for $^3\Sigma_g^+ \rightarrow ^3\Sigma_u^+$ and always remains less than one percent of the latter.

The gain cross section is readily found from the expression $\sigma = \lambda^2 h A / 8\pi$. The peak gain cross section for $v'=0$ of Li_2 $^3\Sigma_g^+$ is $4.5 \times 10^{16} \text{ cm}^2$ at $\lambda = 1.3\mu$. No significant excited-state absorption is likely. Similar calculations are in progress for Na_2 , for which a comparable peak gain cross section near 0.9μ is expected. These alkali dimer continua may well ultimately be useful as tunable near-infrared excimer lasers if a suitable pump can be found.

We have also investigated the predissociation of the $^3\Pi_u$ state by the $^3\Sigma_u^+$ state in Li_2 and Na_2 . This process is pertinent to the question of excited alkali dimer lasers in the $^3\Pi_u$ predissociation acts as a sink to excited state population whenever collisional mixing among the excited manifold is sufficiently rapid. We have calculated the $^3\Pi_u - ^3\Sigma_u^+$

electronic-rotational mixing matrix element for Li_2 and have obtained the predissociation rates for the $^3\Pi_u$ levels. Since the Li_2 $^3\Pi_u$ state is coupled Hund's case (b) due to the very small spin-orbit terms in Li_2 , only half of the six $^3\Pi_u$ fine structure components of a given v and N can be predissociated. All of such levels with $N \geq 10$ from $v'=0$ to the top of the well decay with lifetimes $< 10^{-9}$ sec, with the exception of a few isolated levels near nodes in the oscillating predissociation pattern. The $^3\Pi_u$ predissociation is much weaker in Na_2 due to the lack of a curve crossing below the $^3\Pi_u$ dissociation limit.

f. Excimer Review: Electronic Structure and Radiative Transitions of Excimer Systems.

M. Krauss and F. H. Mies

The review is organized around the different categories of excimer systems. Each category provides an example of one or more of the types of electronic bonding. The ground and excited state electronic structure will be analyzed separately and then the observed spectroscopic transitions coupling these states will be reviewed for the typical cases of rare gas dimer, rare gas-halide, rare gas-group VI, and Group II-Group II excimers. Much briefer discussions will be given of other cases, since no new concepts would be involved and/or there is very little theoretical or experimental information available. In the final section the quantum theory of stimulated emission and absorption in an excimer system will be reviewed. The Franck-Condon factors for the bound-continuum transitions to both the repulsive and flat ground states will be discussed in detail.

IV. Photoionization, Collision-Induced Absorption.

a. Perturbed Rydberg Series: Relationship Between Quantum-Defect and Configuration-Interaction Theory.

F. H. Mies

In this paper we examine the theory of a single Rydberg series which is perturbed by an interloping state. General analytic expressions are presented which apply both to the bound state regions, and to the autoionizing regions above the Rydberg ionization limit. The parameters are expressed in terms of configuration interaction matrix elements, which can be calculated a priori. There is no restriction to weak perturbation theory, and the wavefunction and all its associated properties, such as transition moments, can be extracted. Explicit calculations are presented for the Cd (5s nd) 1D_2 series, perturbed by the Cd (5p²) 1D_2 valence state and excellent results are obtained.

b. Collision - Induced Absorption in Pb.

M. Krauss, W. J. Stevens, H. Basch, P. S. Julienne

Energy curves and transition moments have been calculated for all valence states of Pb and Pb^+ interacting with both He and Xe. These ab initio calculations used relativistic effective core potentials (ECP) that we generated for Xe and Pb. The isotropic piece of the van der Waals interaction was also calculated for all states. Using the energy curves obtained by these methods we concluded that collision-induced absorption is not important for 308 nm (XeCl) pump radiation for either Pb-Xe or Pb-He scattering partners. These energy curves and transition moments will be used as the input for investigating the scattering of Pb with a rare gas in the presence of intense fields from all conceivable viewpoints.

c. Distorted Wave Quenching Cross Sections.

P. S. Julienne and F. H. Mies

We have developed a new distorted wave approximation suitable for use in calculating inelastic scattering cross sections in atom-atom scattering. The approximation is based on the generalized intermediate coupling theory of molecular continuum states developed by Mies. In this theory the exact wavefunction for the two interacting atoms is expanded in a set of electronic-rotational wavefunctions $\{\chi_i\}$ of the diatomic molecule comprised of the two atoms:

$$\psi(\epsilon) = \sum_i \chi_i f_i(R) \quad (1)$$

where χ_i has definite angular momentum J , space-fixed projection M , and parity. The basis $\{\chi_i\}$ can be chosen in any convenient coupling representation (Hund's case). This expansion generates a set of coupled differential equations for the radial functions f_i

$$\sum_i (\langle \chi_j | H | \chi_i \rangle - \epsilon \delta_{ij}) f_i(R) = 0 \quad (2)$$

The off-diagonal couplings in (2) will typically result from electronic-rotation and/or spin-orbit interactions in the molecular Hamiltonian H . A new generalized intermediate coupled basis $\{\chi_\alpha\}$ is then found at each internuclear separation R by diagonalizing the electronic-rotational Hamiltonian at each R .

$$\underline{H}^0 = \underline{M}(R) \underline{H} \underline{M}^{\sim}(R) \quad (3)$$

when $\underline{H}^0$ is diagonal and $\chi_\alpha = \sum_i \chi_i M_{i\alpha}^{\sim}$. This new representation also generates a set of coupled differential equations analogous to (2) for the radial function, y is the expansion

$$\psi(\epsilon) = \sum_\alpha \chi_\alpha g_\alpha(R) \quad (4)$$

Although the original and new set of equations will both lead to the same exact wavefunction (and thus the same transition probabilities) if solved exactly, the new set is quite different in form from the original. Since the electronic-rotational Hamiltonian has been diagonalized, the only coupling between the generalized electronic-rotational states χ_α results from the R-dependence of the unitary transformation coefficients between representations.

A simple distorted wave approximation can be derived in a straightforward manner for the generalized intermediate coupled representation. The result is that the magnitude of the S-matrix element for scattering from scattering from channel α to β is

$$|S_{\alpha\beta}|^{DW} = \frac{\pi\hbar^2}{\mu} f_{\alpha\beta}^\infty T_{\alpha\beta}(R) \left(g_\alpha^0 \frac{d}{dR} g_{\beta\alpha}^0 - g_{\beta\alpha}^0 \frac{d}{dR} g_\alpha^0 \right) dR \quad (5)$$

where g_α^0 represents the energy normalized single channel radial continuum function for potential V_α and

$$T_{\alpha\beta}(R) = (\underline{M}' \underline{\tilde{M}})_{\beta\alpha} = \sum_\gamma M_{\alpha\gamma} \frac{d}{dR} M_{\beta\gamma} \quad (6)$$

is responsible for the off-diagonal coupling.

The approximation (5) has been tested by calculating the quenching cross section for the process

where $M = \text{Hg or Cd}$. The same potential model was used as we used previously to calculate the same cross sections using exact close coupled radial wavefunctions. The DW and exact cross sections are in excellent agreement for quenching of $\text{Hg } ^3P_1$, where the cross section is small and the condition $|S_{10}| \ll 1$ is satisfied for all partial waves and energies.

Although Cd 3P_1 has a large cross section ($K \approx 2 \times 10^{-11} \text{ cm}^3 \text{ sec}^{-1}$) the agreement between exact and DW $|S_{10}|^2$ is excellent for low partial waves and only shows a $\approx 30\%$ difference near the peak value of $|S_{10}|^2 \approx 0.25$.

These preliminary results are very encouraging as to the usefulness of this simple single channel approximation for calculating atom-atom inelastic scattering cross sections in general.

d. Quenching and Predissociation in Group IIb Excimers.

P. S. Julienne

Group IIb homonuclear diatomics have been under consideration as possible excimer lasers. We have used approximate potentials for Zn_2 , Cd_2 , and Hg_2 to investigate the following processes in these species:

(1) The collisional mixing of the 3P $j=0$ and 1 fine structure components due to a collision with a ground state atom of the same kind

$$M(^3P_1) + M(^1S_0) = M(^3P_0) + M(^1S_0),$$

and the closely related process, predissociation of the 1_u state to yield $^3P_0 + ^1S_0$ dissociated atoms.

The potential model is the same as that for Hg_2 given by Mies, Stevens, and Krauss. In this model approximate relativistic potentials (Ω - states) for M_2 are constructed using the non-relativistic molecular potentials and the asymptotic magnitudes of the spin-orbit matrix elements. For the present calculation each of the three species M_2 , $M=\text{Zn}$, Cd , or Hg , was modeled in two ways using the non-relativistic ab initio potentials for Zn_2 and Hg_2 as an approximation to the M_2 non-relativistic potentials.

The model Hg_2 ungerade potentials were used to determine the quenching. The only route by which a 3P_1 atom can be converted to a 3P_0 atom is by collision on the 1_u state correlating with 3P_1 . Although such a collision can give rise to a transition to the 0_u^- state correlating with 3P_0 due to the spin-rotation mixing of the 1_u and 0_u^- states, the two curves do not cross but only approach one another in the left classical turning point region. The same is also true for Cd_2 and Zn_2 .

The coupled equations for the inelastic S-matrix were solved exactly using close coupled wavefunctions and also approximately using a new generalized intermediate coupling single channel approximation. The calculated $^3P_1 \rightarrow ^3P_0$ rate coefficients in units of $10^{-11} \text{ cm}^3 \text{ sec}^{-1}$ molecule are summarized as follows:

Species	Zn		Cd		Hg	
Potential Model =	Zn	Mg	Zn	Mg	Zn	Mg
T = 500K	14	14	5.0	3.2	0.10	3×10^{-5}
750K	17	17	6.8	4.1	0.12	5×10^{-5}
1000K	19	19	8.4	4.7	0.14	9×10^{-5}

The large rate coefficient for Zn is independent of the potential model, whereas the small coefficient for Hg is very sensitive to the model parameters. The Cd coefficient is slightly larger than an approximate measured value, $(1.5 \pm 1) \times 10^{-11} \text{ cm}^3 \text{ sec}^{-1}$ at 600K. The measured value for Hg is $3 \times 10^{-13} \text{ cm}^3 \text{ sec}^{-1}$ near 700K.

The same potential model can be used to obtain the predissociation rates of the bound 1_u levels that lie between the 3P_0 and 3P_1 asymptotes. Each bound 1_u level with a given v and J is doubly degenerate. Only the $(-1)^{J+1}$ parity component of the Ω - doublet can be predissociated. Predissociation of the $(-1)^J$ parity component is rigorously forbidden in all orders in the case of a $1_u - 0_u^-$ interaction. The predissociation rate of the bound levels can be estimated from the S_{01} matrix element for $^3P_1 \rightarrow ^3P_0$ quenching:

$$|_{vJ}(\text{sec}^{-1}) = \frac{\Delta G_v}{h} |S_{01}^J|^2.$$

This expression lends itself to a simple physical interpretation: $\Delta G_v/h$

is the vibrational frequency and $|S_{01}|^2$ is the probability of a transition per vibration extrapolated across the 3P_1 threshold from the 1_u continuum to the 1_u bound levels. Since $|S_{01}^J|^2$ varies approximately as J^2 , there is a large variation in rate from low to high rotational quantum numbers. Except for the lowest rotational levels, the predissociation lifetimes will be in the range 10^{-9} to 10^{-12} sec for Zn_2 , Cd_2 , and Hg_2 . The lifetimes nears the thermal maximum of rotational population will be near 10^{-12} sec for Zn_2 and Cd_2 and near 10^{-10} sec for Hg_2 when the Zn_2 potential model is used. Thus, predissociation will be much faster than radiative or collisional processes for most of the 1_u levels with parity allowed predissociations.

V. Publications

All of the previous sections represent papers in press or being submitted for publication. The papers accepted for publication in 1979 are:

F. H. Mies and P. S. Julienne, IEEE J. Quantum Electron. QE-15, 272 (1979)., "Oscillatory Excimer Emission: An Analytic Model."

M. Krauss and F. H. Mies, Excimer Lasers (Springer, Berlin, 1979) Ed. C. K. Rhodes., "Electronic Structure and Radiative Transitions of Excimer Systems."

P. S. Julienne and M. Krauss, Appl. Phys. Lett., "Role of the $III \frac{1}{2} - II \frac{1}{2}$ Transition in Rare Gas Halide Kinetics."

D. D. Konowalow and P. S. Julienne, Submitted Phys. Rev. Lett., "Spectroscopy of Lithium and Sodium Dimers."

F. H. Mies, to be published, Phys. Rev., "Perturbed Rydberg Series: Relationships Between Quantum-Defect and Configuration Interaction Theory."

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