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Application of a CuBr Laser to the UV Spectroscopy of NaI

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Summary

Many diatomic molecular systems have overlapping potential curves and it is well known that if the electronic states are of the same symmetry then the curves undergo an avoided crossing. Photo-transitions to these states have interesting spectroscopic properties including the Fano profile shapes and very narrow lines above the dissociation limit. This study investigates the non-adiabatic behaviour of such excited states, especially the predissociation of NaI by the ionic-covalent crossing.

A tunable narrow bandwidth (1 GHz) dye laser system pumped by a CuBr laser has been constructed. The frequency doubling of this dye laser radiation to UV was then used to obtain experimental data to investigate the nature of the ionic-covalent crossing of NaI. The high resolution absorption measurements show that the spectrum consists of many more band fragments than that observed with the excitation measurements. Lines in the absorption spectrum of NaI have been assigned and analyzed for the first time. Together with absorption strength determination, this data has been used to demonstrate an inconsistency in the presently accepted molecular potentials. Suggestions for resolving this conflict are presented.

Theoretical investigation was carried out on resonance structure in spectra, including resonance positions, widths and intensities, corresponding to different parameters of the potential surfaces and the coupling strength. Numerical solution of the Schrödinger equations and the complex scaling method were used to investigate the non-adiabatic behaviour of the excited states of diatomic molecules and the model was compared with the results of a semiclassical calculation. Using the assumption that the change of resonance structure from the diabatic to adiabatic limit as the coupling strength increases is smoothly continuous and that the contribution to the resonant state can be considered as part diabatic and part adiabatic, a maximum internal amplitude method is proposed for the location of resonance position and width for a two channel curve crossing system. This technique was used successfully to demon-

strate how resonance structure changes from diabatic to adiabatic limit as the coupling strength changes for a set of model potential curves. The method gives an improved understanding of the origin of the resonance changes in a curve crossing system.