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OPTICAL MOLECULAR SPECTROSCOPY. (U)

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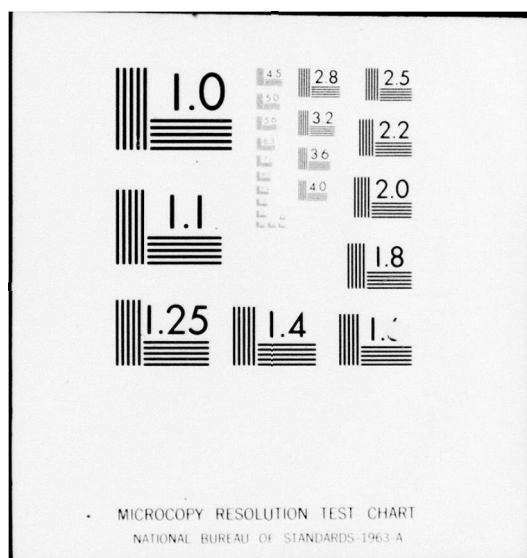
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OPTICAL MOLECULAR SPECTROSCOPY

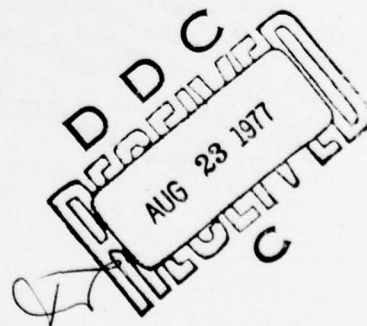
Principal Investigator

Polykarp Kusch

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The B-X spectrum of molecular sodium has been investigated since the birth of molecular spectroscopy where X is the ground $^1\Sigma$ state and B is an excited $^1\Pi$ state. An analysis of this system by the use of laser excited fluorescence spectroscopy has been undertaken by Demtröder, McClintock and Zare and also by Demtröder and Stock. The results of those analyses contain considerable ambiguities that deserve clarification. We have made a major analysis of that spectrum which, in its final form, includes about 13,000 assigned lines. A large extension of the available data occurred through the excitation of many vibrational and rotational levels in the B state by collision between molecules directly excited by the laser and atoms of the buffer gas. Whereas the older analyses identified only a relatively small number of levels in the upper state directly excited by the laser, we have identified more than 1,000 levels in the B state. We reproduce the data through a Dunham Expansion, with a root mean square deviation between observed and calculated line frequencies of about 0.010 cm^{-1} . Our constants will make it possible for investigators to determine the frequency of any line in the B-X spectrum with very high precision. We have, for the first time, established that the centrifugal distortion constant, D_e , agrees with the theoretical value of that constant for an harmonic oscillator to better than 0.25%. We have also demonstrated that the rotational energy cannot readily be described by the conventional expansion. It has not, up to this point, been possible to examine the effect in

detail because of the large correlation between the constants that appear in our Dunham Expansion. For 13,000 lines we required 72 constants to yield the fitting of the data to a formula as described above. We can only believe that the Dunham Expansion is strained to allow the representation of the data. An extended paper dealing with this analysis is now in the process of preparation.

We have examined the spectrum of the A-X system (A is an excited $^1\Sigma$ state) of molecular sodium from the absorption spectrum as observed with the very high resolution and dispersion grating at the Argonne National Laboratories. There are two separable problems associated with the system. The first problem is the perturbation of the lines in the A state through an interaction with a $^3\Sigma$ state of sodium. We have been able to observe the perturbations up to a vibrational quantum number in the A state of about 20. An analysis of these perturbations allows the determination of the constants of the $^3\Sigma$ state to considerable accuracy. A preliminary report of this work has been published by Merrill Hessel and P. Kusch in the *Journal of Chemical Physics*, Vol. 63, No. 9, 1 November 1975. The other problem of interest is the extension of the vibrational quantum numbers in the upper state to very high values which allows a precision determination of the potential curve of the A state. We have been able to identify levels up to a v' of 46. The ground, X state, is admirably delineated in the work as described in the first section of this report. The absorption spectrum which cannot give information about vibrational levels of the ground state in great detail does allow the detailed description of the excited A state. Papers are being prepared to describe our results, both of the perturbations and the extension of the spectrum to very high quantum numbers.

In reading a dissertation by Donald Hsu, the principal investigator in the present grant discovered blunders in the analysis of the A-X system of molecular lithium and a new analysis was made. The principal investigator subsequently learned that Daniel Konowalow at the State University of New York at Binghamton was working on the theory of the A state of lithium. It gives great satisfaction to both the principal investigator and to Professor Konowalow to discover that our new analysis and his theoretical work fit admirably and reinforce each other. A paper on the analysis of the A-X system of Li_2 has been incorporated into an article which has been accepted for publication by the *Journal of Chemical Physics*.

All the work done under the subject contract has been the joint effort of the principal investigator and Dr. Merrill Hessel at the National Bureau of Standards at Boulder, Colorado. The immense amount of calculation that was required in the program was performed at the National Bureau of Standards. The recording of spectra, both fluorescent and absorption, was done at the Argonne National Laboratories at Argonne, Illinois, before the beginning of the present contract. The plates were measured at the National Bureau of Standards.

We believe that we have made definitive analyses of the spectra described above. Further, the style of the analyses will point out some of the traps into which one may readily fall in a detailed analysis of spectra.

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The work carried out under the sponsorship of the subject grant falls in the general field of a critical analysis of the spectra of certain diatomic molecules. An analysis has been made on the B - X spectrum of molecular sodium. About 13,000 lines have been assigned. The data has been reproduced through a Dunham Expansion with a root mean square deviation between observed and calculated line frequencies of about 0.010 inverse centimeters. The constants in the expansion will make it possible for investigators to determine the frequency of any line in the B - X spectrum with very high precision.