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Final Report

NASA Grant NSG 7473

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From

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(NASA-CR-182590) [HIGH RESOLUTION INFRARED
ABSORPTION SPECTRA OF VARIOUS TRACE GASES
PRESENT IN THE UPPER ATMOSPHER OF THE EARTH]
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Background and Objectives

NASA Grant NSG 7473 began July 1, 1978 and ended December 31, 1987. The objective of the work proposed under this grant was to obtain and analyze high resolution infrared absorption spectra of various trace gases present in the upper atmosphere of the earth. The goal of the spectral analysis was to obtain values of absorption line strengths, widths and frequencies of sufficient accuracy for use in upper atmospheric trace gas monitoring.

During the first several years of this grant, high resolution spectra were obtained from two instruments. One was the 0.02 cm^{-1} resolution vacuum grating spectrometer at the Florida State University and the other was the 0.01 cm^{-1} resolution Fourier transform spectrometer at the McMath solar telescope at the Kitt Peak Observatory. Using these instruments, a considerable amount of spectra of Methane and Hydrogen Peroxide were obtained and analyzed. During the latter years of this grant, data taking was halted while efforts were devoted to building a new 0.0025 cm^{-1} resolution vacuum Fourier transform spectrometer. Progress during this phase of the grant then became greatly slowed due to a lack of suitable graduate students in the program. However, the instrument was completed and brought to the point of producing interferograms by the end of the grant period.

Results

Details of the molecular studies completed under this grant are given in the list of publications contained in this report. The following is a brief description of the results obtained.

The first investigation undertaken under this grant was in collaboration with Robert Toth and Linda Brown of the Jet Propulsion Laboratory and Alan Robiette and Jens Lolck of the University of Reading. It consisted of the measurement of the strengths and frequencies of several thousand methane absorption lines in the spectral region 3400 cm^{-1} to 2400 cm^{-1} and the assignment of these lines to the seven strongest vibration - rotation bands in this region. These bands are:

$2V_2$, V_3 , V_1 , V_2+V_4 , $2V_4$, $V_3+V_4-V_4$ and $V_3+V_2-V_2$.

This work was one of the first to assign a substantial number of lines to $2V_2$, V_1 , $V_3+V_4-V_4$ and $V_3+V_2-V_2$ and it also greatly extended the assignments of V_2+V_4 and $2V_4$. A large amount of spectra were taken at several temperatures between -150°C and 25°C and analyzed to obtain the energy of the initial state forming the line. This provided essential data for making quantum assignments. Line intensities as low as $5 \times 10^{-5}\text{ cm}^{-1}/\text{atm-cm}$ were included. By performing a complete analysis of the region, it was possible not only to assign the individual lines, but also to determine the number and approximate strengths of the individual constituents making up unresolved or blended features.

The other molecule investigated during this grant was hydrogen peroxide. Hydrogen peroxide is thought to be an important factor in stratospheric chemistry although present in very low concentration. The spectra of this molecule were studied between 4000 and 3000 cm^{-1} in collaboration with W.B. Olson of the National Bureau of Standards. Because of the low frequency internal rotation in this molecule, the density of lines in its spectrum is very high. Further, the torsional levels including the ground torsional state can not be treated with a set of effective constants for a single torsional level. One of the results of this work was the publication of a quite complete set of rotational levels for the ground torsion - vibration state. From these levels it was shown that the inclusion of an interaction constant coupling the ground state with the first excited torsional state would allow an accurate calculation of the ground state rotational levels. Much of the experimental information on the ground state of hydrogen peroxide was derived from combination differences obtained from assignment of the OH stretching bands V_1 and V_5 for the first time.

While the hydrogen peroxide analysis was in progress, work was begun on the construction of a 0.0025 cm^{-1} resolution Fourier transform spectrometer. The design adopted for the instrument was based on that of the transform spectrometer operated in conjunction with the 4 meter telescope at the Kitt Peak Observatory. This design was chosen for the ease with which the maximum mirror travel could be scaled up to the desired 2 meters. About 3 years were spent in building the basic instrument according to blueprints furnished by Kitt Peak. Initial tests then disclosed that the design did not provide the path difference control needed for operation at infrared wavelengths shorter than about 5 microns. There followed a long period of modifications to improve the path difference control. Ultimately, positioning of the catseye to within 0.01 of the 6238 Angstrom laser wavelength was achieved.

Presently, the instrument is operational with a Calcium Fluoride beamsplitter and Indium Antimonide detector in the region from 2 to 5 microns. The interferograms obtained show a well modulated Central fringe and no problems with fringe loss. Unfortunately, molecular researches proposed during the last grant renewal period could not be performed owing to the long period required to perfect the instrument.

Publications Under NASA Grant NSG 7473

- Extended Line Assignments for the $\nu_3+\nu_4$ Band of $^{12}\text{CH}_4$, R. H. Hunt, L. R. Brown, R. A. Toth and J. W. Brault, *J. Mol. Spectrosc.* 86, 159-169 (1981).
- Line Assignments and Intensities for the $\nu_3+\nu_4-\nu_4$ Band of $^{12}\text{CH}_4$, R. H. Hunt, L. R. Brown, R. A. Toth and J. W. Brault, *J. Mol. Spectrosc.* 86 170-183 (1981)
- Absorption Line Parameters for Methane from 2385 to 3200 cm^{-1} , R. A. Toth, L. R. Brown, R. H. Hunt and L. S. Rothman *Appl. Opt.* 20, 932-935 (1981).
- Line Assignments and Intensities for the $\nu_3+\nu_2-\nu_2$ Band of $^{12}\text{CH}_4$, L. R. Brown, R. A. Toth, R. H. Hunt and J. W. Brault, *J. Mol. Spectrosc.* 89, 528-541 (1981).
- Molecular Constants for the Interacting Upper States of the ν_1 , ν_2 , $2\nu_2$, $\nu_2+\nu_4$ and $2\nu_4$ Bands in $^{12}\text{CH}_4$, J. E. Lolck, A. G. Robiette, L. R. Brown, and R. H. Hunt, *J. Mol. Spectrosc.* 92, 229-245 (1982).
- Measurement and Analysis of the Infrared Absorption Spectrum of the $2\nu_2$ Band of $^{12}\text{CH}_4$, R. H. Hunt, L. R. Brown, J. E. Lolck and A. G. Robiette, *J. Mol. Spectrosc.* 92, 246-256 (1982).
- Analysis of the ν_1 and $\nu_2+\nu_4$ Bands of $^{12}\text{CH}_4$. L. R. Brown, R. A. Toth, A. G. Robiette, J. E. Lolck, R. H. Hunt and J. W. Brault, *J. Mol. Spectrosc.* 93, 317-350 (1982).
- Rotational Constants of the Lowest Torsional Component (OG) of the Ground State and Lowest Torsional Component (1G) of the First Excited Torsional State of Hydrogen Peroxide, W. B. Olson, R. H. Hunt, B. W. Young, A. G. Maki, and J. W. Brault, *J. Mol. Spectrosc.* 127 12-34 (1988).