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QUARTERLY

R E P O R T

by

THE OHIO STATE UNIVERSITY  
RESEARCH FOUNDATION

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To: DEPARTMENT OF THE NAVY  
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On: STRUCTURAL AND THERMODYNAMIC PROPERTIES OF  
POLYATOMIC MOLECULES AT ELEVATED TEMPERATURES

For the period: 1 April 1963 - 30 June 1963

Submitted by: David White  
Department of Chemistry

Date: 6 August 1963

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STRUCTURAL AND THERMODYNAMIC PROPERTIES OF  
POLYATOMIC MOLECULES AT ELEVATED TEMPERATURES

The analysis of the thermodynamic and spectral data of the molecular species  $\text{LiO}$ ,  $\text{Li}_2\text{O}$  and  $\text{Li}_2\text{O}_2$  has been completed. The results were presented at the Symposium of Molecular Structure and Spectroscopy in Columbus, Ohio. A complete report of the work entitled "The Infrared Spectra, Structures and Thermodynamics of Gaseous  $\text{LiO}$ ,  $\text{Li}_2\text{O}$ , and  $\text{Li}_2\text{O}_2$ ," has been submitted for publication.

The analysis of the infrared spectrum of  $\text{Al}_2\text{O}^{16}$ ,  $\text{Al}_2\text{O}^{18}$  has been completed during the period and a report is now under preparation. As previously indicated this molecule appears to have an open structure in  $C_{2v}$  symmetry. The isotopic shifts are consistent with a bond angle in the range 140 to 160 degrees.

Some preliminary mass spectrometric and matrix isolation studies have been completed on the vapors in equilibrium with solid sodium peroxide at elevated temperatures. We have positively identified the molecular species  $\text{Na}_2\text{O}$ ,  $\text{NaO}$  in the vapor phase and possibly the peroxide form of  $\text{Na}_2\text{O}_2$ . The infrared spectra of the vapors trapped in solid Krypton matrices show bands which from the magnitude of the frequencies appear to be due to sodium oxygen stretches in the molecular species  $\text{Na}_2\text{O}$  and  $\text{NaO}$ .

During this report period we have completed the fabrication assembly and testing of the equipment to determine the true band widths of simple diatomic molecules trapped in solid rare gas matrices at low temperatures. A specially designed dewar utilizing a Air Products Miniature Joule-Thomson Liquifier will be employed in these experiments. This will be coupled to the high resolution grating spectrometer ( $0.04$  to  $0.05 \text{ cm}^{-1}$ ) of Professor Rao in the Department of Physics.

Measurements of the infrared spectrum of matrix isolated  $\text{B}_2\text{Cl}_4$  using the prism instruments have been completed. An analysis of the results indicated the necessity of examination of some of the bands under conditions of higher resolution. These experiments are just getting under way.

Investigator \_\_\_\_\_ Date \_\_\_\_\_

Supervisor David White Date 8/7/63

For The Ohio State University Research Foundation

*Acting*  
Executive Director Thomas E. Davis Date 8/8/63