# State of California AIR RESOURCES BOARD

### Resolution 01-32

September 20, 2001

Agenda Item No.: 01-7-3

WHEREAS, the Air Resources Board has been directed to carry out an effective research program in conjunction with its efforts to combat air pollution, pursuant to Health and Safety Code sections 39700 through 39705;

WHEREAS, a research proposal, number 2498-221, entitled "Impact of NO<sub>X</sub> Surface Reactions on the Formation of Particles, Ozone, and the Development of Control Strategy Options," has been submitted by the University of California, Irvine;

WHEREAS, the Research Division staff has reviewed and recommended this proposal for approval; and

WHEREAS, the Research Screening Committee has reviewed and recommends for funding:

Proposal Number 2498-221 entitled "Impact of NO<sub>X</sub> Surface Reactions on the Formation of Particles, Ozone, and the Development of Control Strategy Options," submitted by the University of California, Irvine, for a total amount not to exceed \$400,003.

NOW, THEREFORE BE IT RESOLVED, that the Air Resources Board, pursuant to the authority granted by Health and Safety Code section 39703, hereby accepts the recommendation of the Research Screening Committee and approves the following:

Proposal Number 2498-221 entitled "Impact of NO<sub>X</sub> Surface Reactions on the Formation of Particles, Ozone, and the Development of Control Strategy Options," submitted by the University of California, Irvine, for a total amount not to exceed \$400,003.

BE IT FURTHER RESOLVED, that the Executive Officer is hereby authorized to initiate administrative procedures and execute all necessary documents and contracts for the research effort proposed herein, and described in Attachment A, in an amount not to exceed \$400,003.

I hereby certify that the above is a true and correct copy of Resolution 01-32, as adopted by the Air Resources Board.

Marie Kavan, C	lerk of the Board

#### **ATTACHMENT A**

"Impact of NO<sub>X</sub> Surface Reactions on the Formation of Particles, Ozone, and the Development of Control Strategy Options"

## **Background**

Nitrogen oxides (NO<sub>x</sub>) play a fundamental role in the creation of ozone, particles, and other pollutants in the atmosphere through photochemical reactions with volatile organic compounds. In addition to these gas-phase processes, heterogeneous reactions of NO<sub>x</sub> are also important in the creation of pollutants. Two such reactions that are likely to be important in urban areas, yet are poorly understood and are not included in current airshed models, are the hydrolysis of NO<sub>2</sub> to produce HONO and HNO<sub>3</sub>, and the generation of NO<sub>2</sub> from NO and HNO<sub>3</sub>. The first reaction creates HONO, which plays a pivotal role in the initiation of smog formation at dawn. The second reaction transforms deposited HNO<sub>3</sub> into photochemically active (gas-phase) NO<sub>x</sub>. This latter reaction counters the widely accepted viewpoint that HNO<sub>3</sub> is an end product that takes NO<sub>x</sub> out of the atmosphere. An understanding and accurate parameterization of these reactions is necessary to assess different pollution control strategies and air quality modeling studies. Preliminary modeling studies suggest that these heterogeneous reactions may have a significant effect on peak levels of ozone and particulates.

# **Objective**

The objectives of this research are to determine, using a combination of laboratory and modeling studies, 1) the mechanism and rate of HONO formation from the hydrolysis of NO<sub>2</sub>, 2) the mechanism and rate at which HNO<sub>3</sub> is converted back into photochemically active forms, 3) the possible photoenhancement of these reactions, and 4) the impact of these reactions on ozone and particulate formation in urban areas.

#### Methods

A newly constructed attenuated total reflectance-long path infrared apparatus (ATR-LPIR) will be used to simultaneously monitor the infrared spectrum of the gas phase and a liquid film in a reaction cell. Nitric acid,  $N_2O_4$ , nitric and nitrite ion will be measured in a thin water film on an ATR crystal (composed of Ge, KRS-5, ZnSe, or AMTIR). The thickness of the water layer will be varied by using air of various relative humidities. Photosensitivity of the reactions will be investigated using a Xe lamp, which simulates solar radiation with suitable filters. In addition to these measurements, a long-path gas cell with Fourier transform infrared spectrometry will be used as an independent method to investigate the possible photoenhancement of heterogeneous  $NO_X$  reactions.

# **Expected Results**

A comprehensive chemical reaction model will be constructed from the experimentally determined mechanisms and rate constants. Airshed modeling studies will be carried out for different NO<sub>x</sub>/VOC scenarios.

## Significance to the Board

The information gained in this project will improve our understanding of the reactions critical to accurately predicting the effect of NO<sub>X</sub> controls on PM and ozone levels. Thus, it will improve our understanding of the processes involved in the formation of secondary pollutants that pose health risks and degrade California's visibility. The information will also be used to improve the chemical mechanisms used in the ARB's attainment modeling for the State Implementation Plan.

#### **Contractor:**

University of California, Irvine

## **Contract Period:**

27 months

# **Principal Investigator (PI):**

Professor Barbara Finlayson-Pitts

### **Contract Amount:**

\$400.003

# Cofunding:

none

### **Basis for Indirect Cost Rate:**

The State and University of California System have agreed to a ten percent indirect cost rate.

## Past Experience with this Principal Investigator:

Professor Finlayson-Pitts did an excellent job on a previous ARB contract and she was very cooperative in responding to requests from ARB staff. Her previous project produced a large amount of excellent quality science.

## Prior Research Division Funding to the University of California, Irvine:

Year	2001	2000	1999
Funding	\$ 0	\$ 215,000	\$ 501,999

# **BUDGET SUMMARY**

University of California, Irvine

Impact of NO<sub>x</sub> Surface Reactions on the Formation of Particles, Ozone, and the Development of Control Strategy Options

DIRE	CT COSTS AND BENEFITS			
1.	Labor and Employee Fringe Benefits	\$	272,556	
2.	Subcontractors	\$	0	
3.	Equipment	***	0	
4.	Travel and Subsistence	\$	6,000	
5.	Electronic Data Processing	\$	0	
6.	Reproduction/Publication	\$	0	
7.	Mail and Phone	\$	0	
8.	Supplies	\$	65,544 <sup>1</sup>	
	Analyses	\$	0	
10.	Miscellaneous	<u>\$</u>	<u> 21,000</u>	
	Total Direct Costs		\$365,100	
	RECT COSTS	Φ.	04.000	
1.	Overhead	\$	34,903	
2.	General and Administrative Expenses	\$ \$ \$	0	
3.	Other Indirect Costs	Þ	0	
4.	Fee or Profit	<u>\$</u>	0	
	Total Indirect Costs		<u>\$34,9</u>	<u>03</u>
TOTAL PROJECT COSTS				

<sup>&</sup>lt;sup>1</sup>Funds will be used for the purchase of disposable supplies such as optical components, gases, solvents, chemical, glassware, stockroom and office supplies to be used on this project.