State of California AIR RESOURCES BOARD

Resolution 03-31

December 11, 2003

Agenda Item No.: 03-10-5

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 2538-232, entitled "Identification and Atmospheric Reactions of Polar Products of Selected Aromatic Hydrocarbons," has been submitted by the University of California, Riverside;

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 2538-232 entitled "Identification and Atmospheric Reactions of Polar Products of Selected Aromatic Hydrocarbons," submitted by the University of California, Riverside, for a total amount not to exceed \$49,999.

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 2538-232 entitled "Identification and Atmospheric Reactions of Polar Products of Selected Aromatic Hydrocarbons," submitted by the University of California, Riverside, for a total amount not to exceed \$49,999.

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 as described in Attachment A, in an amount not to exceed \$49,999.

I hereby certify that the above is a true and						
correct copy of Resolution 03-31, as adopted						
by the Air Resources Board.						
Stacey Dorais, Clerk of the Board						

ATTACHMENT A

"Identification and Atmospheric Reactions of Polar Products of Selected Aromatic Hydrocarbons"

Background

Aromatic hydrocarbons are a significant portion of anthropogenic emissions of VOCs, and form major components of vehicle exhaust, emissions from combustion processes, and evaporative emissions from industrial processes and solvent usage. These compounds play a central role in the formation of secondary pollutants, such as ozone and secondary organic aerosol (SOA), which is due not only to their high emission rates but also to their generally high reactivity in the atmosphere. Estimates indicate that the oxidation of aromatic hydrocarbons is a major contributor to ozone formation on local and regional scales, and, because of the relatively high yield of low volatility products, to the formation of SOA. In contrast to their importance in the production of secondary pollutants, information concerning reaction rates and detailed mechanisms leading to these products is limited. This incomplete knowledge is due to several factors: ringopening reaction pathways are complex and depend sensitively on the experimental conditions (e.g. NOx concentrations); multifunctional oxygenated compounds are difficult to measure, especially as a function of time as needed in kinetic studies; the multifunctional products are generally highly reactive.

Objective

The objectives of this project are to identify and measure the rates of formation of dicarbonyl and hydroxycarbonyl compounds that are produced by hydroxyl radical-initiated reactions of aromatic hydrocarbons. In addition, the rates of reaction of the carbonyl-containing products with hydroxy radicals will be measured, along with photolysis rates and products of these processes.

Methods

A variety of techniques will be used to both identify and measure the concentrations of chemical species within large volume Teflon chambers: derivatization will be done with Solid-Phase Micro Extraction (SPME) fibers, which allows on-fiber derivatization of carbonyl-containing products; identification of compounds will be made by combined gas chromatography-mass spectrometry (GC-MS) and gas chromatography-flame ionization detection (GC-FID) analysis.

Expected Results

Using these methods, time-concentration measurements of carbonyl products will be taken (approximately every five minutes during a reaction); this data will allow accurate determination of the rate constants for both hydroxyl radical-initiated reactions and photolysis of the products.

Significance to the Board

The primary benefit provided by this project would be accurate kinetic and mechanistic data for atmospheric reactions of aromatic hydrocarbons, highly reactive compounds

that form ozone and PM2.S₁ which will assist in the formulation of more accurate atmospheric chemistry models of air pollution, including the formation of secondary organic aerosols. Such models will also help in the development of effective air pollution control strategies and in assessments of the human health risks associated with aromatic hydrocarbons.

Contractor:

University of California, Riverside

Contract Period:

12 months

Principal Investigators (PIs):

Roger Atkinson and Janet Arey

Contract Amount:

\$49,999

Cofunding:

None

Basis for Indirect Cost Rate:

The State and UC System have agreed to a ten percent indirect cost rate.

Past Experience with this Principal Investigator:

These Principal Investigators have performed very successfully in all previous contracts with the ARB, which span over 15 years. Their work has addressed the atmospheric chemistry of a variety of volatile organic compounds and has led to improved rates and mechanisms in models.

Prior Research Division Funding to UCR:

Year	2002	2001	2000	
Funding	\$0	\$467,736	\$894,890	

BUDGET SUMMARY

University of California at Riverside

"Identification and Atmospheric Reactions of Polar Products of Selected Aromatic Hydrocarbons"

DIRECT COSTS AND BENEFITS							
1.	Labor and Employee Fringe Benefits	\$	35,304				
2.	Subcontractors	\$	0				
3.	Equipment		0				
4.	Travel and Subsistence		1,000				
5.	Electronic Data Processing		0				
6.	Reproduction/Publication		0				
7.	Mail and Phone	\$	200				
8.	Supplies	\$	8,500				
9.	Analyses	\$	0				
10.	Miscellaneous	\$	450				
	Total Direct Costs			\$ 45,454			
INDIRECT COSTS							
1.	Overhead	\$	4,545				
2.	General and Administrative Expenses	\$	0				
3.	Other Indirect Costs	\$	0				
4.	Fee or Profit	\$	0				
	Total Indirect Costs			\$ 4,545			
TOTAL PROJECT COSTS				<u>\$ 49,999</u>			