

Summary- (RG/99/C/05)

Title of Project: Identification of the Involvement of Singlet Oxygen, $O_2(^1\Delta_g)$, in Atmospheric Oxygenation of Polycyclic Aromatic Hydrocarbons

Institution: Department of Chemistry, University of Ruhuna

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Date of Completion: -----

Scientific Background and Scope

$O_2(^1\Delta_g)$ is one of the reactive forms of molecular oxygen. The formation of $O_2(^1\Delta_g)$ by photosensitization in polluted atmospheres is a viable process since some of the pollutants can act as sensitizers. Oxy-PAH's, which were isolated from atmospheric samples of urban areas, have exhibited carcinogenic/mutagenic activity. PAH's are constantly released to atmospheres by incomplete combustion of fossil fuel at high temperature. It is important to understand the processes by which oxy-PAH's are formed in the atmosphere. Therefore, we undertook to study the involvement of $O_2(^1\Delta_g)$ in atmospheric oxygenation of PAH's.

Objectives:

To generate $O_2(^1\Delta_g)$ in gas phase; To establish a method to quantify gas phase $O_2(^1\Delta_g)$; To react PAH's with $O_2(^1\Delta_g)$; To react PAH's with oxygen under simulated atmospheric conditions; To carry out quenching experiments.

Experimental Methods:

- **Model PAH:** Benz[a]anthracene, B[a]A
- **Gas phase $O_2(^1\Delta_g)$ formation by photosensitization:** By passing mixtures of nitrogen and oxygen in different ratios through Rose Bengal-coated glass tubes under illumination.

- **Quantification of $O_2(^1\Delta_g)$:** By GC analysis of TME-OH obtained by reducing TME-OOH which is produced in the reaction of $O_2(^1\Delta_g)$ with tetramethylethylene (TME).
- **HPLC detection of B[a]A, and 7,12-dione of B[a]A:** C_8 reversed phase column was used in a Hitachi single pump HPLC equipped with a UV-vis detector and a data processor.
- **GC detection of TME and TME-OH:** For pack column GC analysis, a stainless column packed with stationary phase SP1000 was used in a Hitachi GC equipped with a FID and a data processor. Ultra pure nitrogen gas with a flow rate of 30 mL/min was used as the carrier gas. Air and ultra pure hydrogen were used for the FID. The injection volume was 10 μ L.
- Attempts were also made to convert the GC to accommodate capillary columns.

Results and Discussion:

- Flow generator apparatus consisting of the photochemical exposure chamber, traps photochemical reactor, gas flow controllers, valves, gas bubblers, and tubings was constructed.
- **HPLC analysis of benz[a]anthracene, B[a]A, and B[a]A-7, 12-dione:** Mobile phase: 20:80 mixture of water : acetonitrile with a flow rate of 1.0 mL/min.

<u>Compound</u>	<u>Retention time / min</u>
B[a]A	8.00 \pm 0.50
B[a]A-7,12-dione	12.00 \pm 0.50

- **GC analysis of TME and TME-OH:** The detection of tetramethylethylene, TME, was successful in GC analysis with our SP1000-packed column as detected by Flame Ionisation Detector. However, TME-OH was not detected. Experiments to form $O_2(^1\Delta_g)$ were repeatedly carried out and their reaction mixtures were subjected to GC analysis, but no TME-OH was detected. The reason could be so low levels of TME-OH formed that pack column GC is not sensitive enough to detect TME-OH at low

concentrations. Though attempts were made to convert the existing GC to accommodate capillary columns it was failed. Meantime the Research Assistant resigned.

Conclusions and Recommendations:

No major conclusions or recommendations can be made because a research assistant was unable to be found to continue the project after the first two research assistants resigned.