ESR STUDY OF RADIATION
DAMAGE IN PYRIMIDINES

Progress Report
for Period August 1, 1975 - April 1, 1976

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TECHNICAL PROGRESS REPORT

Aug. 1, 1975 - April 1, 1976

ABSTRACT

The primary objective of this project is to develop general mechanisms for radiation damage to biomolecules using substituted pyrimidines as a model system. Results this year include a single crystal ESR study of 5-ethyl-5-isopropylbarbituric acid, development of the k-band microwave bridge, dose response measurements on methylated barbituric acid derivatives, and synthesis of several specifically deuterated uracil derivatives.

TECHNICAL PROGRESS REPORT

The primary objective of this project is to investigate radiation damage to biomolecules using substituted pyrimidines as a model system. During the first nine months of the current contract year progress was made in the following areas:

1. Publication of the work on 5-ethyl-5-isoamylbarbituric acid. Abstraction of the isoamyl group at room temperature is preceded by hydrogen abstraction from that group observed at 77°K. This mechanism follows a pattern observed previously in our laboratory for ethyl abstraction. (Radiat. Res., in press, 1976).
2. Analysis of 5-ethyl-5-isopropylbarbituric acid is nearing completion. The free radical observed is formed by abstraction of hydrogen from a terminal methyl of the isopropyl group. A report of this work will be presented at an upcoming meeting (24th Meeting of the Radiation Research Society, San Francisco, June 1976).
3. Single crystal studies at 77°K using the k-band microwave bridge and cavity constructed under this contract are progressing slowly. Modifications of the original design have been undertaken to allow work at lower microwave power as power saturation has been a problem. Relaxation times in some barbituric acid derivatives under study are apparently longer than expected from similar compounds.

4. Initial experiments with the digital signal averager and processor recently acquired under this contract showed promise. A component malfunction (which was corrected by the manufacturer only this week) has prevented extensive use. We have a large backlog of nearly finished dose-response experiments which are awaiting completion using the signal processor to integrate the ESR spectra.
5. ESR analysis of dialuric acid and benzalbarbituric acid, synthesized during the last contract year, has begun. The free radical structures cannot be identified from polycrystalline spectra, so we are attempting to grow single crystals. These compounds are important to the development of our general model of radical formation so that extended efforts at crystallization are being applied to these difficult compounds.
6. Additional 5-deuterated and 6-deuterated uracil derivatives have been synthesized. These will be used to study hydrogen addition mechanisms and whether the site of addition depends upon having an anionic precursor.