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## Abstract

Polycyclic aromatic hydrocarbons (PAHs) are known byproducts of anthropogenic sources including incomplete combustion of fossil fuels. They are known to be teratogenic, mutagenic and carcinogenic. This study investigated the spectral properties of fluoranthene and 3-nitrofluoranthene using NMR, UV-Vis and infrared techniques. The acquisition of spectral data provides a means to identify these compounds in mixtures and can be used which to develop model formulae for quantitation. A 2-D NMR method (HMQC ) was used for assigning $^{13}C$ peaks. The infrared spectrum for 3-nitrofluoranthene showed characteristic strong absorption peaks at 1323 and 1516 cm$^{-1}$ assigned to symmetric/asymmetric nitro stretches, respectively. UV–vis characterization showed a bathochromic shift. This finding supports a degree of nitro group planarity with the fluoranthene moiety; in agreement with the finding that planar molecules exhibit greater mutagenicity when introduced into biological systems. The structure, then, is of paramount importance in understanding the molecule's biological effects on cells.

## Purpose

1. Nitro PAHs exhibit greater mutagenicity than their parent compounds.

2. Acquire and assign the spectral fingerprints of 3-nitrofluoranthene.

3. Correlate structure to observed biological properties.

** The acquisition of spectra helps to identify these compounds in mixtures/ or atmosphere. The identification of spectral properties helps to develop and evaluate analytical methods such as FT-IR/MS/GC coupling by providing standards.

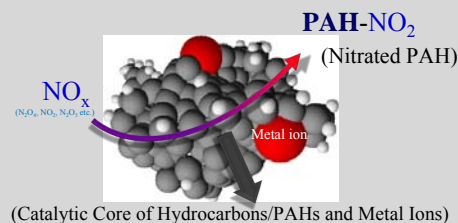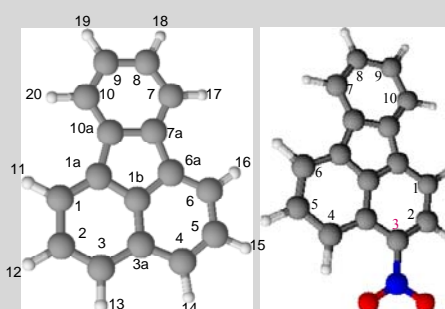## Examples of PAH Sources and Effects

## Common PAHs

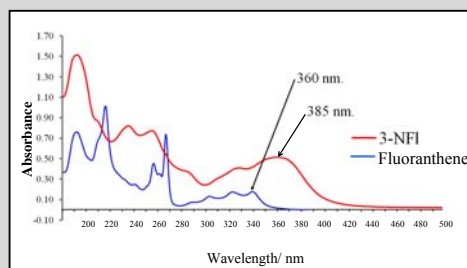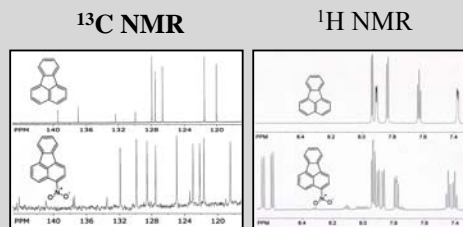Triphenylene          Coronene          Pyrene

## Method of Nitration

PAH-$NO_2$
(Nitrated PAH)

$NO_x$
(N$_2$O$_4$, NO$_2$, N$_2$O$_3$ etc.)

Metal ion

(Catalytic Core of Hydrocarbons/PAHs and Metal Ions)

## Structures Studied

## RESULTS: (a) UV Vis Spectra

360 nm.
385 nm.
3-NFl
Fluoranthene

Wavelength/ nm

## RESULTS:  (b) NMR

### $^{13}C$ NMR

### $^{1}H$ NMR

## HMQC
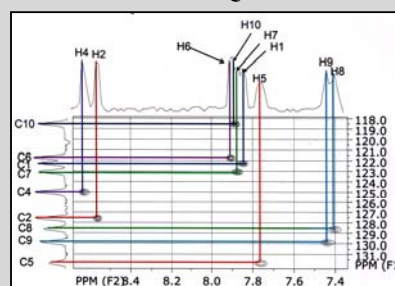
## (b) NMR

### $^{13}C$ NMR Assignments (ppm.)

C8 -128.7  C9 -130.0
C7 -123.1
C10 -118.4
C6 -121.6
C5 -132.0   C1 -122.2
C4 -125.0   C2 -127.6
C3 -144.2

| Position | ($\delta$, ppm) |
|---|---|
| 1 | 122.2 |
| 2 | 127.6 |
| 3 | 144.2 |
| 4 | 125.0 |
| 5 | 132.0 |
| 6 | 121.6 |
| 7 | 123.1 |
| 8 | 128.7 |
| 9 | 130.0 |
| 10 | 118.4 |

## (c) Infrared

3-NFl
Fluoranthene

1516 cm$^{-1}$ (asymmetric stretch)
1323 cm$^{-1}$ (symmetric stretch)

% Transmittance

cm$^{-1}$
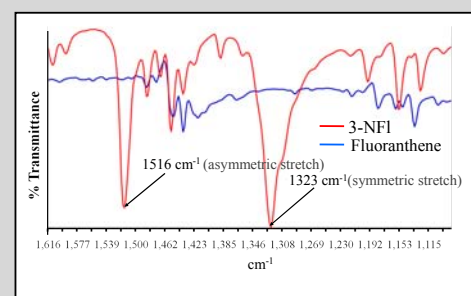
| $\nu_{asym}(NO_2)$ | $\nu_{sym}(NO_2)$ |
|---|---|
| 1516 cm$^{-1}$ | 1323 cm$^{-1}$ |

## Conclusions

1. The NMR values for $^{13}C$ have been successfully assigned and correlated.

2. The UV-Vis spectra illustrate the planar orientation of the nitro group due to is a shift to longer wavelengths.

3. The groundwork has been laid for a better structural understanding of the nitrated fluoranthenes.

## Further Work

1. To assign  tertiary $^{13}C$ NMR chemical shifts for 3-nitrofluoranthene by other 2-D methods e.g. HMBC.

2. To synthesize/ characterize other nitrated fluoranthenes.

3. To test the biological potencies of synthesized nitrated fluoranthenes using transgenic cell lines.

## References

1) Squadrito G. et. al., *Chem Res. Toxicol*., (1990) 3, 231-235
2) Onchoke K, *Polycyc. Aromat. Compds*, (2008), 28,193-212
3) Greibrokk T., et. al., *Acta. Chem. Scand*., 1983, Ser. B B37, 833-844.

## Acknowledgments