

# How is Naphthalene Degraded in the Environment?

Jack Robertson, b1016629

## 1. Aims and Implications

To synthesise a key compound in the anaerobic degradation of naphthalene.

To understand the importance of anaerobic naphthalene degradation

To explain the roles of microbial enrichment culture N47 in anaerobic naphthalene degradation.

Can N47 be used to aid a greener clean up of naphthalene pollution?

## 3. The Trouble with Naphthalene

Naphthalene is hazardous to human health and natural habitats. Acute exposure of humans to naphthalene by inhalation, ingestion or dermal contact is associated with haemolytic anaemia, damage to the liver and neurological damage. The compound is suspected of having carcinogenic effects.

Naphthalene originates from anthropogenic sources and can make its way into the environment via man-made industrial processes as well as oil spills.

The substance is contained in crude oil and it is the smallest PAH. Naphthalene readily partitions into water, so oil spills into oceans can lead to naphthalene deposits.

Anoxic conditions deep in the ocean mean that degradation via dioxygenases cannot take place.

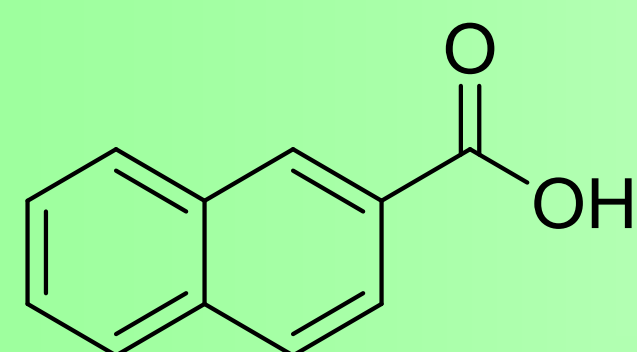
These problems lead us into research on anaerobic degradation pathways, which is of potential importance in the battle against environmental pollution.

## Naphthalene-2-carboxylic Acid (1)

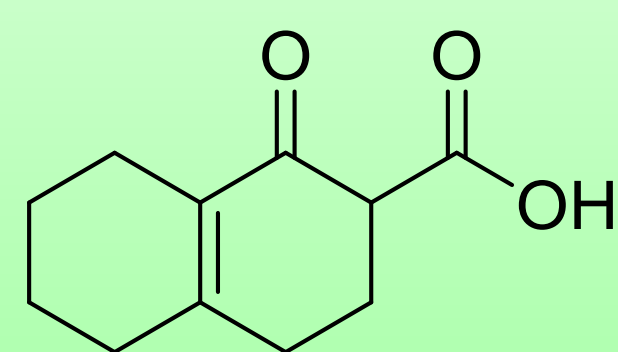
A common intermediate in N47-mediated degradation of naphthalene and 2-methylnaphthalene is naphthalene-2-carboxylic acid.

This compound is necessary for investigations into anaerobic naphthalene degradation as explained in the N47 section.

Compound 2 is proposed as a possible degradation product from naphthalene-2-carboxylic acid.



1



2

Acknowledgements– I would like to thank Newcastle University for this opportunity. And I would like to thank Professor Bernard Golding and Dr Andrey Zaytsev for their continued support and guidance throughout this Project.

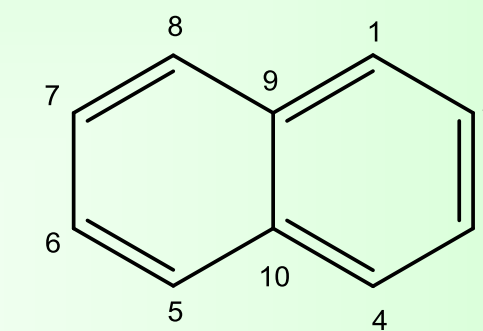
## 2. Naphthalene Structure

Naphthalene is the simplest polycyclic aromatic hydrocarbon (PAH).

Aromatic compounds: obey Hückel's rule ( $4n+2$   $\pi$  electrons, cyclic conjugated, planar molecule).

Naphthalene consists of two 6 carbon aromatic rings.

Each carbon position is numbered as shown.



## 4. Culture N47

This microbial cluster is anaerobic naphthalene degrading when enriched in sulphate-reducing conditions.

Can grow on naphthalene and some other naphthalene derivatives (2-methyl, 2-carboxylic acid, 1-carboxylic acid) where these species are the sole carbon and energy source for the culture.

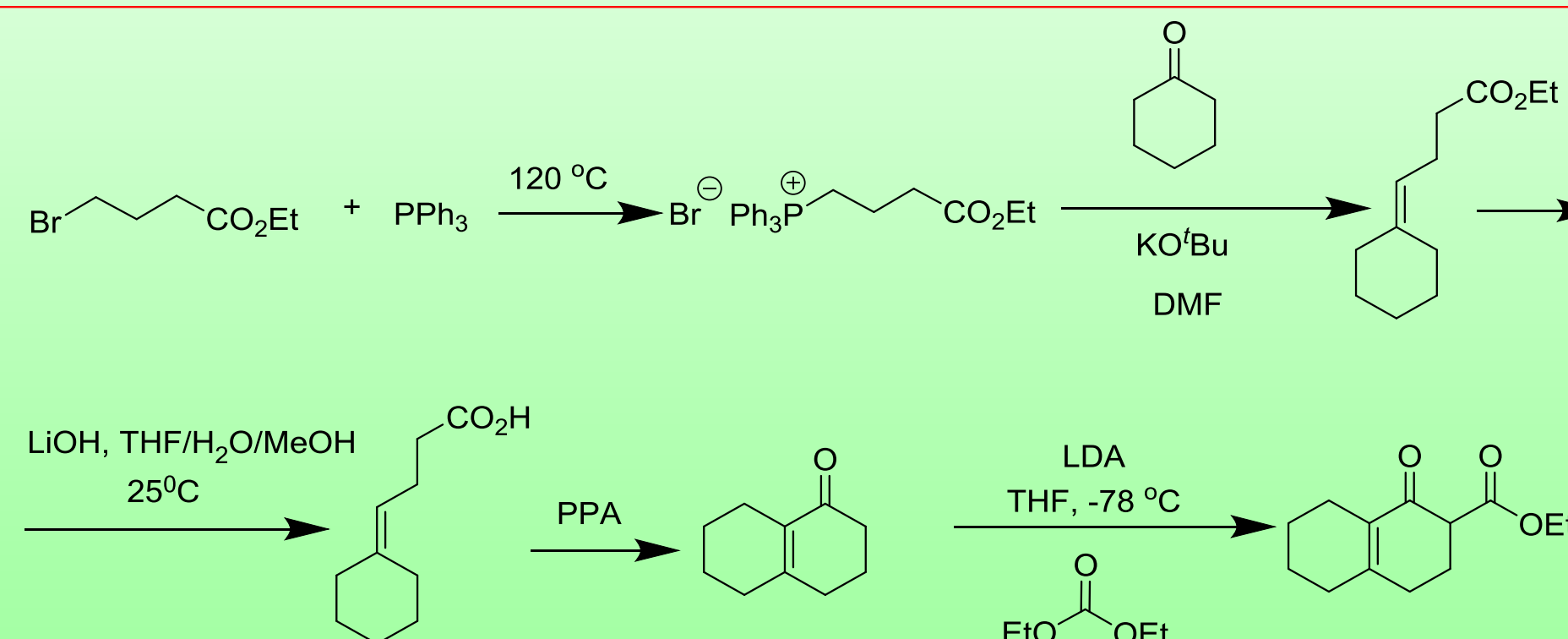
N47 degrades naphthalene through various intermediates, but always via naphthalene-2-carboxylic acid.

Scheme 1 highlights the likely reduction path N47 forces naphthalene to take resulting in compound 2.

Scheme 1 shows that reaction (ii) is a 4-electron reduction of naphthalene-2-carboxylic acid. This reaction is believed to be catalysed by naphthoyl-CoA reductase.

Reaction (iii) is a 2-electron reduction and finally reaction (iv) gives a key metabolite in the anaerobic degradation pathway (Compound 2) that can be synthesised.

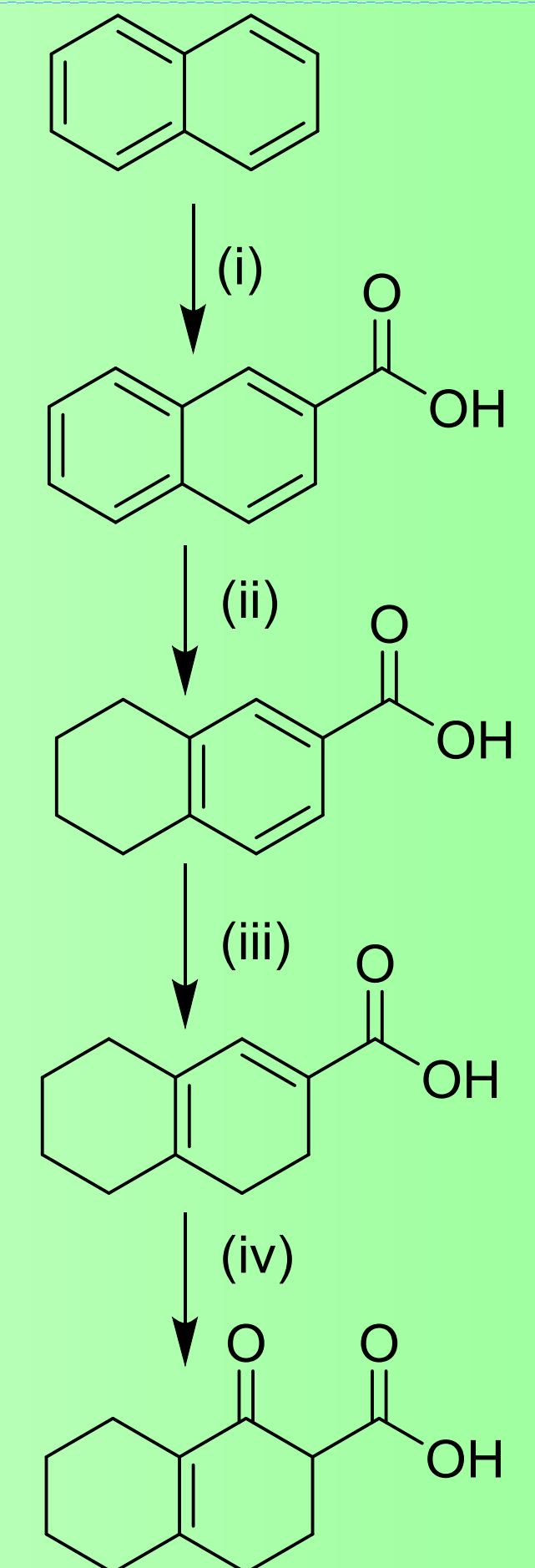
## Synthetic approach to compound 2 (ethyl ester)



DMF *N,N*-Dimethylformamide, THF Tetrahydrofuran, PPA Polyphosphoric acid, LDA Lithium Diisopropyl amide

## Scheme 1

Metabolic pathway from naphthalene to compound 2



## References

- Toxicological Profile for Naphthalene* (Update). Public Health Service, U.S. Department of Health and Human Services, Atlanta, GA. 1995.
- Chang W, Um Y & Holoman TRP (2006) Polycyclic aromatic hydrocarbon (PAH) degradation coupled to methanogenesis. *Biotechnology Letters* **28**: 425-430.
- Eberlein C, Golding BT, et al. (2013) ATP-dependent/-independent enzymatic ring reductions involved in the anaerobic catabolism of naphthalene. *Environmental Microbiology* **6**: 1832-1841
- Bergmann FD, et al. RU (2011) Identification of new enzymes potentially involved in anaerobic naphthalene degradation by the sulfate-reducing enrichment culture N47. *Archives of Microbiology* **193**: 241-250.