

# Organic chemistry lab determination of the structure of a natural product in anis...

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Task DETERMINATION OF THE STRUCTURE OF A NATURAL OIL PRODUCT IN ANISE OIL The purpose of this experiment is to isolate the anise oil major component and unveil its structure and identity with use of IR spectroscopy and determination of melting point.

### 1. Reaction mechanism

The phase-transfer catalysis is aided by Aliquat 336. Organophilic and hydrophilic characters in the reaction are being transferred to the aqueous and organic phases. The anions of the reactants and the products are transferred across the interfacial region into the organic phase as an integral phase-transfer cation-anion pair.

Organic phase  $R-Y + Q+X^- \rightleftharpoons R-X + Q+Y^-$

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Interfacial

region

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Aqueous phase

$NaY + Q+X^- \rightleftharpoons NaX + Q+Y^-$

The major component in anise oil has the chemical formula  $C_{10}H_{12}O$ . It is a hydrogen deficient component having less hydrogen atoms than would be required for every carbon atom to have the maximum amount of attached hydrogen atoms. The molecule's index of hydrogen deficiency is 10. This implies that there are 5 rings or double bonds in the structure. Each one

would then compensate for the two of the hydrogen atoms that are not there (Lehman, p. 292-294).

Upon catalytic hydrogenation of anise oil, a saturated compound with a chemical formula  $C_{10}H_{20}O$ , it points to the original structure to be containing four pi bonds, since eight hydrogen atoms were added (Lehman, p. 292-294).

## 2. Meaning of ortho, meta, and para

Ortho - a combining form used in the name of an acid in a given series of acids containing the most water.

An ortho substitution has a frequency range of 735-770 ( $cm^{-1}$ ).

Meta - a prefix denoting the least hydrated of a series.

Meta substitution has a frequency range of 750-810 and 630-730( $cm^{-1}$ ).

Para - a combining form designating the (1, 4) position in the benzene ring.

Para substitution has a frequency range of 790-840 ( $cm^{-1}$ ) (Lehman, p. 291-297).

## 3. Possible effects of :

### A) absence of Aliquat 336

Aliquat 336 functions as phase transfer catalyst, it provides green chemistry procedures. If it was not added, the experiment would not have been environmentally friendly due to the hazardous wastes produced during the chemical reactions.

B) The Ph 7 of the filtered reaction mixture indicates a neutral mixture. It points to addition of insufficient 6M HCL which was required to make the reaction mixture acidic. The reaction mixture ought to have turned brown after addition of anise oil and heat, which turns white in addition of  $NaSOH_3$ .

## References

Lehman, John. Multiscale Operational Organic Chemistry. Prentice Hall, New Jersey, 2002.