Synthesis of multi-functional isoprene hydroxy hydroperoxide components of fine particulates with implications on human health

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Background

- **Isoprene is the largest non-methane volatile organic compound (VOC) emitted into the atmosphere, with around 440-600 TgC yr^{-1} of isoprene being emitted annually by biogenic sources, specifically vegetation.**

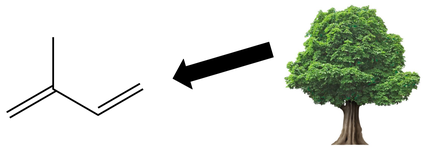

Figure 1: Isoprene and its source

- **Isoprene rapidly reacts with hydroxyl radicals (•OH) in the troposphere.**
- **A class of these oxidation products are known as isoprene hydroxy hydroperoxides (ISOPOOHs). The ISOPOOH that is the target of this synthesis is 1,2-ISOPOOH, as that is the major oxidation product of ISOPOOH formed in the atmosphere.**
- **The need for synthetic standards helps to understand the fate of ISOPOOH in the atmosphere due to continuous oxidation.**
- **The synthesis performed here utilizes an already published method that will involve the opening of 2-methyl-2-vinyloxirane using hydrogen peroxide (H_2O_2) in an acid-catalyzed reaction.**

Methods

- **Dried etheric H_2O_2 reacted w/ 2-methyl-2-vinyloxirane and catalytic phosphomolybdic acid (PMA)**
- **After overnight mixing, excess solvent was removed using a rotary evaporator. Any excess H_2O_2 that remained was removed using a freeze drier.**
- **Product was isolated using silica gel column and sand in preparation for column chromatography with solvent system of 90:10 dichloromethane:acetone.**
- **The analyte was collected and characterized using ^1H and ^{13}C NMR.**

Acknowledgements

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Structures and Reactions

Figure 2: 1,2-ISOPOOH

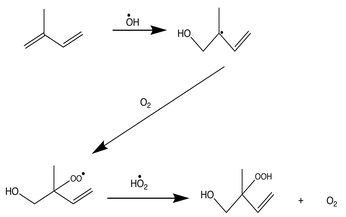

Figure 3: 1,2-ISOPOOH formation in atmosphere

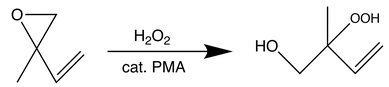

Figure 4: Synthetic reaction of 1,2-ISOPOOH formation

Results

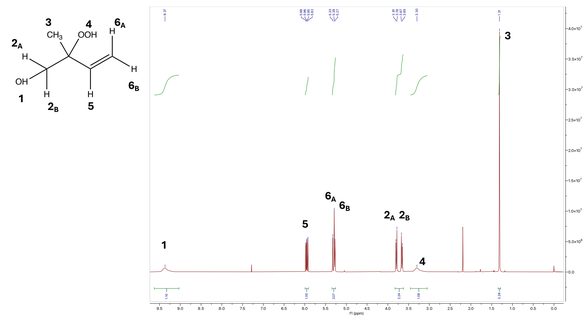

Figure 5: ^1H NMR and structure elucidation of 1,2-ISOPOOH sample

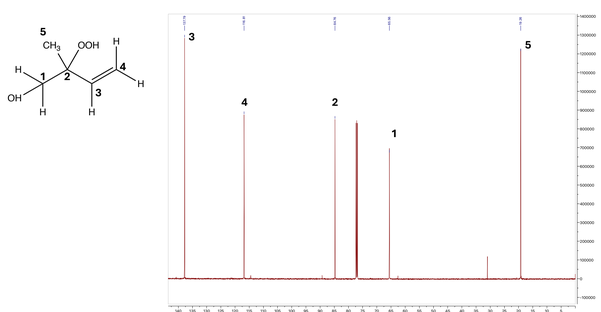

Figure 6: ^{13}C NMR and structure elucidation of 1,2-ISOPOOH sample

Discussion

- **^1H NMR generated is consistent with ^1H NMRs of 1,2-ISOPOOH present in published literature**
- **In both ^1H NMR and ^{13}C NMR, there is a residual peak which is assigned to acetone, which was used as a solvent when purifying the analyte,**
- **To produce cleaner signals, more time must be taken while conducting column chromatography to ensure that only the analyte of interest is eluted.**

Future Directions

- **Isoprene oxidation research is a prominent topic in environmental atmospheric chemistry, and there are many directions that this project may proceed.**
- **Isoprene is emitted in greater amounts in warmer climates. Isoprene emissions are expected to increase in the coming decades due to climate change. Thus, further research can be conducted on atmospheric transformation in the wake of increased isoprene oxidation.**
- **Another highly researched topic relating to isoprene is its relation to human toxicology. Isoprene oxidation products are known to condense onto particles and form secondary organic aerosols (SOAs). SOAs contribute to total atmospheric mass of $PM_{2.5}$.**
- **It has been widely known that inhaling SOAs has led to increased oxidative stress in the respiratory system. The synthesized product can be used in comparative studies to see how the oxidative stress induced by 1,2-ISOPOOH-majority SOAs are different than that of other isoprene products.**
- **Additionally, while much investigation has taken place regarding the toxicological effects of ISOPOOH in the respiratory system, there is a limited amount of research of the direct toxicological changes that 1,2-ISOPOOH induces in other body systems. Research can be conducted on how 1,2- ISOPOOH affects the bloodstream and the epithelial skin tissue, especially regarding people that live in predominantly urban areas.**

References

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